



STIC Search Report

Biotech-Chem Library

STIC Database Tracking Number: 206718

TO: Rei-Tsang Shiao
Location: REM-5A10/5C18
Art Unit: 1626
Tuesday, November 21, 2006
Case Serial Number: 10/749806

From: Les Henderson
Location: Biotech-Chem Library
REM-1B61
Phone: (571)272-2538

leslie.henderson@uspto.gov

Search Notes

Results can also be viewed via SCORE. <http://es/ScoreAccessWeb/>

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STIC SEARCH RESULTS FEEDBACK FORM

Biotech-Chem Library

Questions about the scope or the results of the search? Contact **the searcher or contact:**

Mary Hale, Information Branch Supervisor
571-272-2507 Remsen 1 A51

Voluntary Results Feedback Form

➤ I am an examiner in Workgroup: Example: 1610

➤ Relevant prior art **found**, search results used as follows:

- ☐ 102 rejection
- ☐ 103 rejection
- ☐ Cited as being of interest.
- ☐ Helped examiner better understand the invention.
- ☐ Helped examiner better understand the state of the art in their technology.

Types of relevant prior art found:

- ☐ Foreign Patent(s)
- ☐ Non-Patent Literature
(journal articles, conference proceedings, new product announcements etc.)

➤ Relevant prior art **not found**:

- ☐ Results verified the lack of relevant prior art (helped determine patentability).
- ☐ Results were not useful in determining patentability or understanding the invention.

Comments:

Drop off or send completed forms to STIC/Biotech-Chem Library Remsen Bldg.

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Scientific and Technical Information Center

SEARCH REQUEST FORM

Requester's Full Name: Robert (Kerby) Shiao Examiner #: 79521 Date: 1/06/06
Art Unit: 1626 Phone Number: 2-0707 Serial Number: 10/749 806
Location (Bldg/Room#): REM (Mailbox #): 5401 Results Format Preferred (circle): PAPER DISK

15018

To ensure an efficient and quality search, please attach a copy of the cover sheet, claims, and abstract or fill out the following:

Title of Invention: Process for producing phthalic anhydride
Inventors (please provide full names): Watanabe et al.

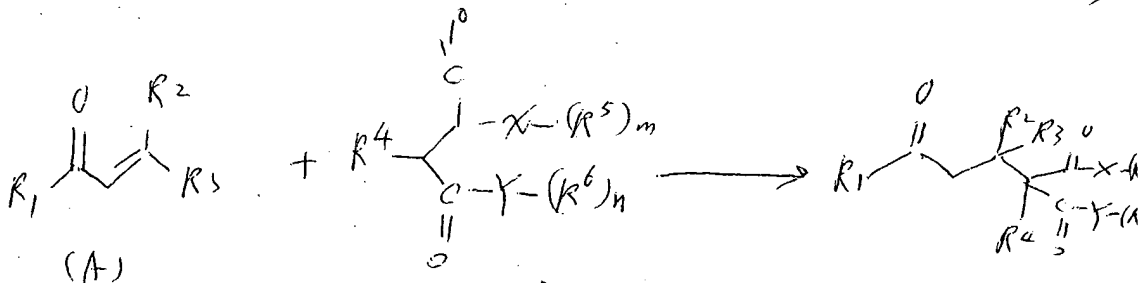
Earliest Priority Date: _____

Search Topic:

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc., if known.

For Sequence Searches Only Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.

2. Search a process of making epd(c) by (see claim 1)



(B)

* $R^1 \sim R^6$ are sub.

(C)

A. X, Y is a bond, O, S, N or P.

* $R_1 \sim R_6$ are sub

* $R^1/R^2, R^1/R, R^2/R^3$ may

form a ring

2. Search a process making (R)-3-[bis(ethoxycarbonyl)methyl]-cyclopentanone by reacting (see ex. 8, 9)
hexamethylbenzene + 2-cyclopentanone \rightarrow product.

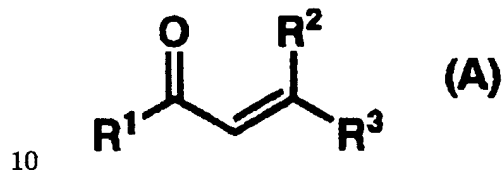
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[Chem. 3]

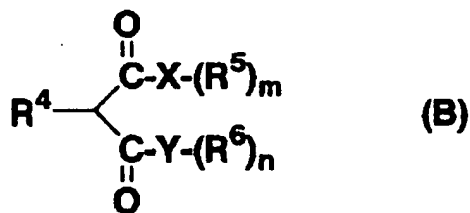


may form
ring

a substituent, or a straight-chain or branched C1 to C20 alkoxy group, and R⁴ and R⁵, R⁴ and R⁶, or R⁵ and R⁶ may be bonded to each other to form a ring; X and Y independently denote a single bond, an oxygen atom, a sulfur atom, a ~~nitrogen atom, or a phosphorus~~ atom; and m and n are independently 1 or 2; when X and/or Y is a single bond, an oxygen atom, or a sulfur atom, m and/or n is 1, and when X and/or Y is a nitrogen atom or a phosphorus atom, m and/or n is 2) by reacting a compound represented by general formula (A) [Chem. 1]



(in the formula, R¹, R², and R³ have the same meaning as above) and a compound represented by general formula (B) [Chem. 2]



15 (in the formula, R⁴, R⁵, R⁶, X, Y, m, and n have the same meaning as above) with an asymmetric metal complex obtained from an optically active nitrogen-containing compound and a complex of a metal of group VIII of the periodic table.

2. The process for producing an optically active compound according to Claim 1, wherein X and Y of compound (B) according to Claim 1 are both oxygen atoms.

3. The process for producing an optically active compound according to Claim 1, wherein X of compound (B) according to Claim 1 is an oxygen atom and Y is a single bond, or X is a single bond and Y is an oxygen atom.

chromatography (hexane/acetone = 90/10, SiO₂) to give 213 mg (99% yield) of the title compound. The optical purity was measured by HPLC (CHIRALPAK AS manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 80 : 20, flow rate 1.0 mL/min, detection at 210 nm) and it was found to be 89 %ee.

(Example 8)

Production of (R)-3-[bis(ethoxycarbonyl)methyl] cyclopentanone

Under an atmosphere of argon, 12.6 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (hexamethylbenzene), 84 μ L (1.0 mmol) of 2-cyclopentenone, 152 μ L (1.0 mol) of diethyl malonate, and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO₂) to give 233 mg (96% yield) of the title compound. After this was converted into an ethylene ketal derivative by the same procedure as in Example 3, the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 97 : 3, flow rate 0.5 mL/min, detection at 210 nm) and it was found to be 96 %ee.

(Example 9)

Production of (S)-3-[bis(ethoxycarbonyl)methyl] cyclopentanone

Under an atmosphere of argon, 24.0 mg (0.04 mmol, S/C = 50) of RuH[(R,R)-Tsdpen] (1,3,5-trimethylbenzene), 168 μ L (2.0 mmol) of 2-cyclopentenone, 304 μ L (2.0 mmol) of diethyl malonate, and 2 mL of acetone were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO₂) to give 462 mg (95% yield) of the title compound. After this was converted into an ethylene ketal derivative by the same procedure as in Example 3,

the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd., hexane : 2-propanol = 97 : 3, flow rate 0.5 mL/min, detection at 210 nm) and it was found to be 91 %ee.

5 (Example 10)

Production of 3-[1,1-bis(methoxycarbonyl)ethyl] cyclopentanone

Under an atmosphere of argon, 12.6 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (hexamethylbenzene), 84 μ L (1.0 mmol) of 2-cyclopentenone, 133 μ L (1.0 mmol) of dimethyl methylmalonate, 10 and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 24 hours. This solution was purified by flash column chromatography (hexane/acetone = 90/10, SiO₂) to give 54 mg (24% yield) of the title compound. The optical purity was measured by HPLC (CHIRALPAK AS manufactured by Daicel Chemical 15 Industries, Ltd., hexane : 2-propanol = 80 : 20, flow rate 1.5 mL/min, detection at 210 nm) and it was found to be 76 %ee.

(Example 11)

Production of 3-[bis(methoxycarbonyl)methyl]-4,
4-dimethylcyclopentanone

20 Under an atmosphere of argon, 12.3 mg (0.02 mmol, S/C = 50) of Ru[(S,S)-Tsdpen] (1,2,3,4,5-pentamethylbenzene), 122 μ L (1.0 mmol) of 4,4-dimethyl-2-cyclopentenone, 114 μ L (1.0 mmol) of dimethyl malonate, and 1 mL of 2-methyl-2-propanol were placed in a 20 mL Schlenk tube and stirred at 40°C for 48 hours. This solution 25 was purified by flash column chromatography (hexane/acetone = 90/10, SiO₂) to give 141 mg (58% yield) of the title compound. After they were converted into an ethylene ketal derivative by the same procedure as in Example 3, the optical purity was measured by HPLC (CHIRALCEL OD manufactured by Daicel Chemical Industries, Ltd.,



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Bib Data Sheet

CONFIRMATION NO. 6518

SERIAL NUMBER 10/749,806	FILING DATE 12/31/2003 RULE	CLASS 558	GROUP ART UNIT 1626	ATTORNEY DOCKET NO. 60542(49811)
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APPLICANTS

Masahito Watanabe, Soka-shi, JAPAN;
 Kunihiro Murata, Soka-shi, JAPAN;
 Takao Ikariya, Tokyo, JAPAN;

** CONTINUING DATA *****

** FOREIGN APPLICATIONS *****
 JAPAN 2003-9786 01/17/2003
 JAPAN 2003-71368 03/17/2003

IF REQUIRED, FOREIGN FILING LICENSE GRANTED
 ** 03/23/2004

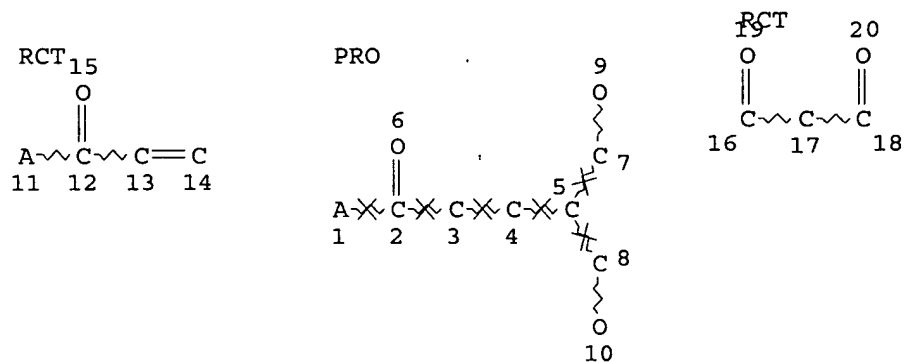
Foreign Priority claimed 35 USC 119 (a-d) conditions met Verified and Acknowledged	<input checked="" type="checkbox"/> yes <input type="checkbox"/> no <input type="checkbox"/> yes <input type="checkbox"/> no <input type="checkbox"/> not after allowance Examiner's Signature <i>[Signature]</i> Initials <i>[Initials]</i>	STATE OR COUNTRY JAPAN	SHEETS DRAWING 0	TOTAL CLAIMS 9	INDEPENDENT CLAIMS 1
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ADDRESS
 EDWARDS & ANGELL, LLP
 P.O. Box 9169
 Boston, MA
 02209

TITLE
 Process for producing optically active compound

FILING FEE RECEIVED	FEES: Authority has been given in Paper No. _____ to charge/credit DEPOSIT ACCOUNT No. _____ for following:	<input type="checkbox"/> All Fees <input type="checkbox"/> 1.16 Fees (Filing) <input type="checkbox"/> 1.17 Fees (Processing Ext. of time) <input type="checkbox"/> 1.18 Fees (Issue)
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L10 STR



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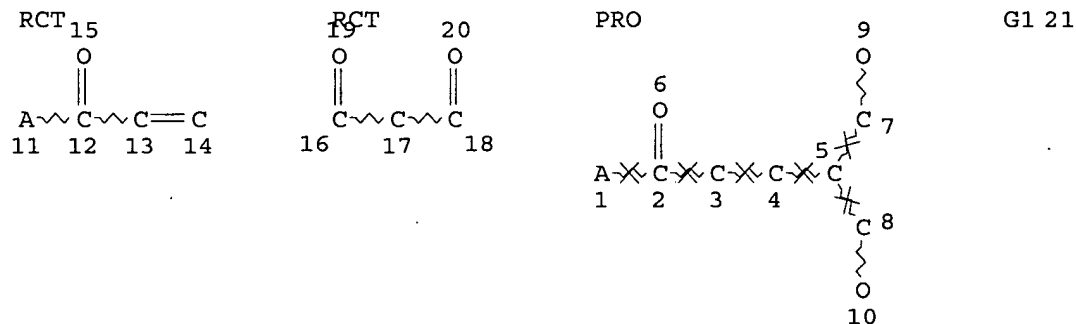
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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

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NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE

L15 629 SEA FILE=CASREACT SSS FUL L10 (2897 REACTIONS)
L17 STR



Fe @22 Co @23 Ni @24 Ru @25 Rh @26 Pd @27 Os @28 Ir @29

Pt @30

VAR G1=22/23/24/25/26/27/28/29/30

NODE ATTRIBUTES:

NSPEC IS RC AT 22
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NSPEC IS RC AT 26
NSPEC IS RC AT 27

11/21/2006

Shiao 10/749,806

11/21/2006

NSPEC IS RC AT 28
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CONNECT IS E1 RC AT 9
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 30

STEREO ATTRIBUTES: NONE

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)

100.0% DONE 31 VERIFIED 31 HIT RXNS 7 DO
CS
SEARCH TIME: 00.00.02

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L20 ANSWER 1 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 136:37336 CASREACT

TITLE: Tandem anionic Michael addition/radical
cyclizations: a new and efficient strategy for
the synthesis of functionalized cyclopentanes

AUTHOR(S): Jahn, Ullrich

CORPORATE SOURCE: Institut fur Organische Chemie, TU
Braunschweig, Braunschweig, D-38106, Germany

SOURCE: Chemical Communications (Cambridge, United
Kingdom) (2001), (17), 1600-1601

CODEN: CHCOFS; ISSN: 1359-7345

PUBLISHER: Royal Society of Chemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 24-4 (Alicyclic Compounds)

ABSTRACT:

The combination of anionic Michael addition of lithium ester enolates with
radical 5-exo cyclizations through single electron transfer (SET)
oxidation gives highly functionalized cyclopentanes.

SUPPL. TERM: electron transfer cyclization Michael addn ester
enolate

INDEX TERM: Electron transfer
(preparation of functionalized cyclopentanes via
tandem anionic Michael addition/radical cyclization)

INDEX TERM: Cyclization
(radical; preparation of functionalized cyclopentanes
via tandem anionic Michael addition/radical
cyclization)

INDEX TERM: Addition reaction
Michael reaction
(stereoselective; preparation of functionalized
cyclopentanes via tandem anionic Michael
addition/radical cyclization)

INDEX TERM: 2564-83-2, TEMPO
ROLE: CAT (Catalyst use); RCT (Reactant); RACT
(Reactant or reagent); USES (Uses)
(prepn of functionalized cyclopentanes via tandem
anionic Michael addition/radical cyclization)

INDEX TERM: 11077-24-0, Ferrocenium hexafluorophosphate
ROLE: CAT (Catalyst use); RCT (Reactant); RACT
(Reactant or reagent); USES (Uses)
(preparation of functionalized cyclopentanes via
tandem anionic Michael addition/radical cyclization)

INDEX TERM: 94-41-7 1462-12-0 5292-53-5 377752-09-5
377752-10-8 377752-11-9 377752-12-0
377752-13-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of functionalized cyclopentanes via
tandem anionic Michael addition/radical cyclization)

INDEX TERM: 377752-26-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation of functionalized cyclopentanes via
tandem anionic Michael addition/radical cyclization)

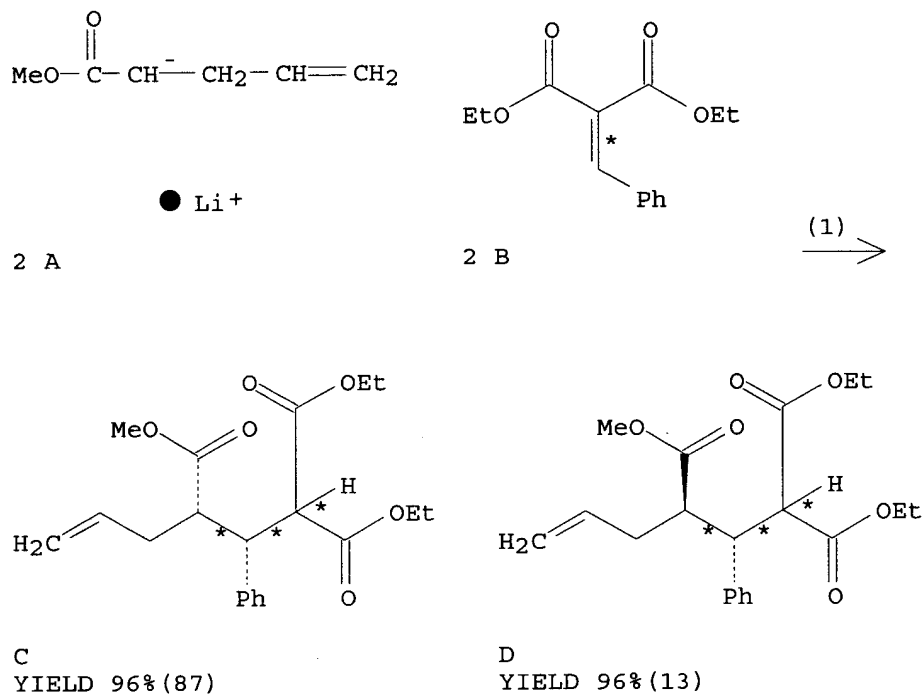
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377752-60-8P 379738-76-8P 379738-77-9P
379738-78-0P 380153-16-2P 380153-18-4P
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(preparation of functionalized cyclopentanes via
tandem anionic Michael addition/radical cyclization)

REFERENCE COUNT: 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR
THIS RECORD.

REFERENCE(S): (1) Bernardi, A; Gazz Chim Ital 1995, V125, P539
CAPLUS
(2) Boger, D; J Org Chem 1997, V62, P8875 CAPLUS
(3) Cohen, T; Tetrahedron 1993, V49, P7931 CAPLUS
(4) Curran, D; Comprehensive Organic Synthesis 1991,
V4, P715
(5) Curran, D; Comprehensive Organic Synthesis 1991,
V4, P779
(6) Curran, D; Stereochemistry of Radical Reactions
1996
(7) Fischer, H; Angew Chem, Int Ed 2001, V40, P1340
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(8) Giese, B; Org React 1996, V48, P301 CAPLUS
(9) Gorobets, E; Usp Khim 2000, V69, P1091
(10) Heathcock, C; Modern Synthetic Methods 1992,
V6, P1 CAPLUS

- (11) Jahn, U; Chem Commun 1998, P209 CAPLUS
 (12) Marek, I; J Chem Soc, Perkin Trans 1 1999, P535 CAPLUS
 (13) Melikyan, G; Org React 1997, V49, P427 CAPLUS
 (14) Oare, D; J Org Chem 1990, V55, P157 CAPLUS
 (15) Oare, D; Top Stereochem 1989, V19, P227 CAPLUS
 (16) Sibi, M; J Am Chem Soc 1999, V121, P7517 CAPLUS

RX(1) OF 17 2 A + 2 B ==> C + D



RX(1) RCT A 377752-09-5, B 5292-53-5

STAGE(1)

RGT E 680-31-9 HMPT

SOL 109-99-9 THF

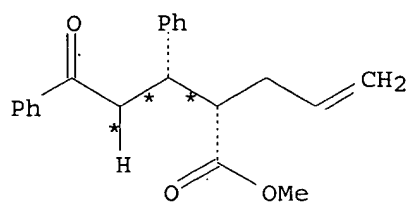
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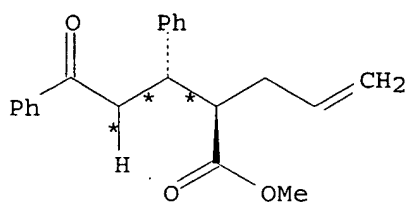
PRO C 377752-14-2, D 377752-15-3

NTE stereoselective

RX(2) OF 17 2 A + 2 B ==> D + C



I
YIELD 84% (88)



J
YIELD 84% (12)

RX(3) RCT A 377752-09-5, H 94-41-7

STAGE(1)

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SOL 109-99-9 THF

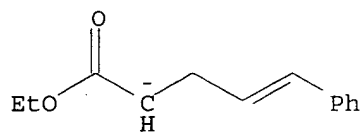
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PRO I 377752-16-4, J 377752-17-5

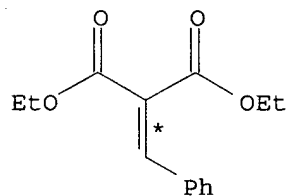
NTE stereoselective

RX(4) OF 17 2 K + 2 B ==> L + M



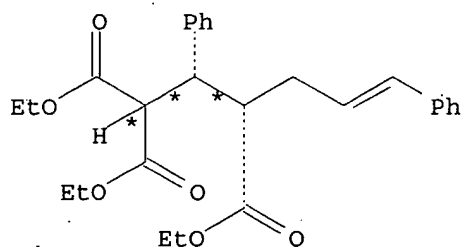
● Li⁺

2 K

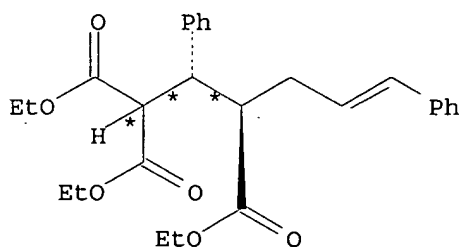


2 B

(4) →

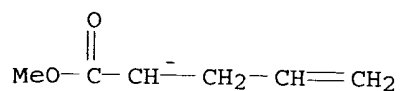


L
YIELD 95% (90)

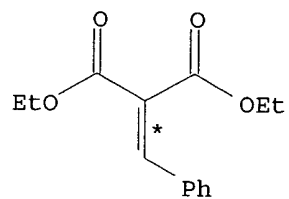


M
YIELD 95% (10)

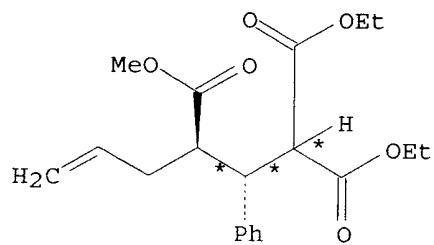
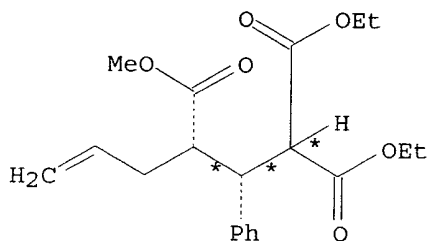
RX(4) RCT K 377752-10-8, B 5292-53-5



2 A



2 B

(2) \longrightarrow D
YIELD 58%(65)C
YIELD 58%(35)

RX(2) RCT A 377752-09-5, B 5292-53-5

STAGE(1)

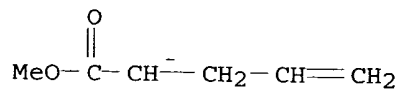
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STAGE(2)

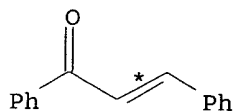
RGT F 7732-18-5 Water

PRO D 377752-15-3, C 377752-14-2

NTE stereoselective

RX(3) OF 17 2 A + 2 H \implies I + J

2 A



2 H

(3) \longrightarrow

STAGE(1)

RGT E 680-31-9 HMPT

SOL 109-99-9 THF

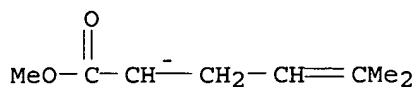
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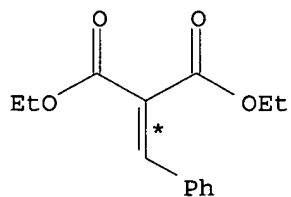
PRO L 377752-18-6, M 377752-19-7

NTE stereoselective

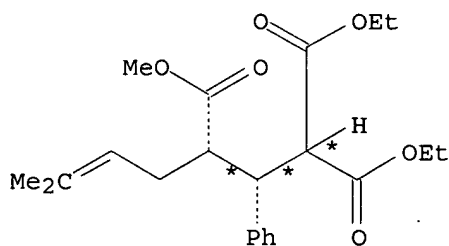
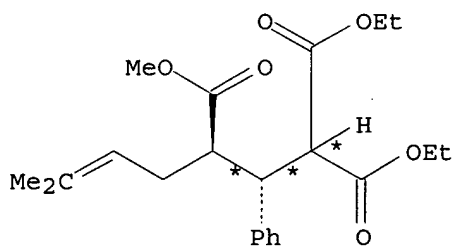
RX(5) OF 17 2 N + 2 B ==> O + P



2 N



2 B

(5) \longrightarrow O
YIELD 77%(92)P
YIELD 77%(8)

RX(5) RCT N 377752-12-0, B 5292-53-5

STAGE(1)

RGT E 680-31-9 HMPT

SOL 109-99-9 THF

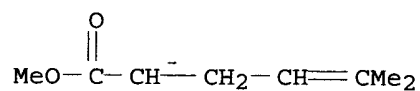
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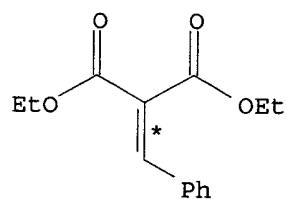
PRO O 377752-20-0, P 377752-21-1

NTE stereoselective

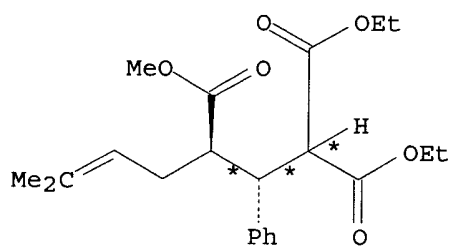
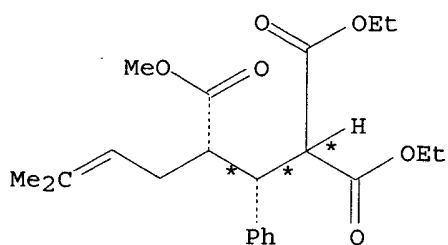
RX(6) OF 17 2 N + 2 B ==> P + O



2 N



2 B

(6) \longrightarrow P
YIELD 90% (69)O
YIELD 69% (31)

RX (6) RCT N 377752-12-0, B 5292-53-5

STAGE (1)

SOL 109-99-9 THF

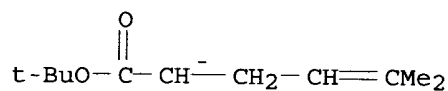
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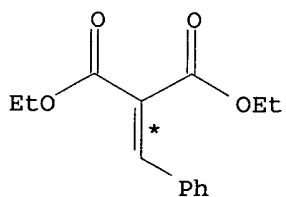
PRO P 377752-21-1, O 377752-20-0

NTE stereoselective

RX (7) OF 17 2 Q + 2 B ==> R + S

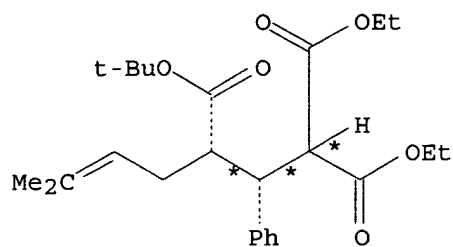


2 Q

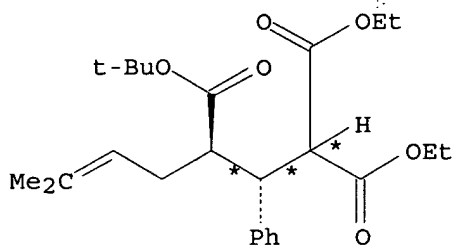


2 B

(7) \longrightarrow



R
YIELD 93% (92)



S
YIELD 93% (8)

RX (7) RCT Q 377752-13-1, B 5292-53-5

STAGE (1)

RGT E 680-31-9 HMPT

SOL 109-99-9 THF

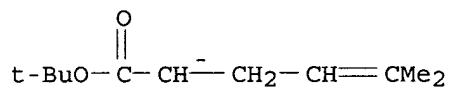
STAGE (2)

RGT F 7732-18-5 Water

PRO R 377752-22-2, S 377752-23-3

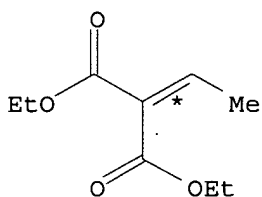
NTE stereoselective

RX (8) OF 17 2 Q + 2 T ==> U + V



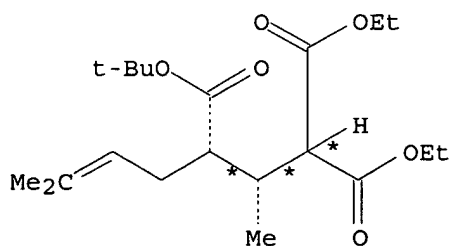
● Li⁺

2 Q

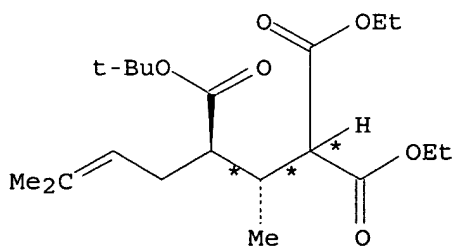


2 T

(8) →



U
YIELD 92% (82)



V
YIELD 92% (18)

RX(8) RCT Q 377752-13-1, T 1462-12-0

STAGE(1)

RGT E 680-31-9 HMPT

SOL 109-99-9 THF

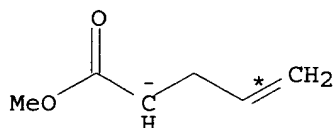
STAGE(2)

RGT F 7732-18-5 Water

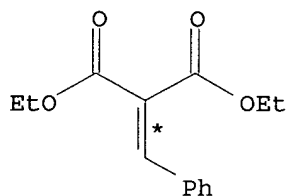
PRO U 377752-24-4, V 377752-25-5

NTE stereoselective

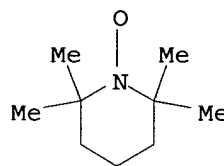
RX(9) OF 17 A + B + W ==> X

● Li⁺

A

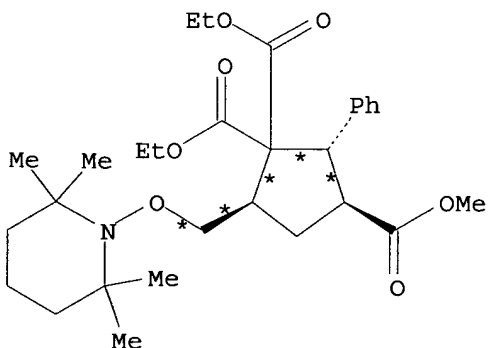


B



W

(9) →



X

YIELD 71%

RX(9) RCT A 377752-09-5

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT W 2564-83-2

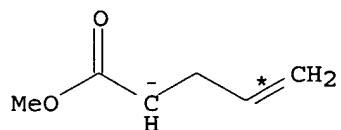
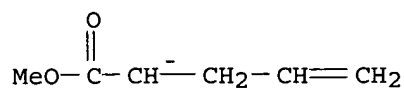
RGT AA 11077-24-0 Ferrocenium PF₆

STAGE(4)

RGT F 7732-18-5 Water

PRO X 377752-26-6

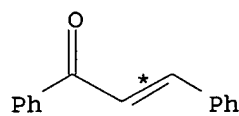
RX(10) OF 17 5 A + 5 H + 5 W ==> AC + AD + AE + AF +
AG



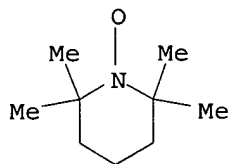
4 A



A

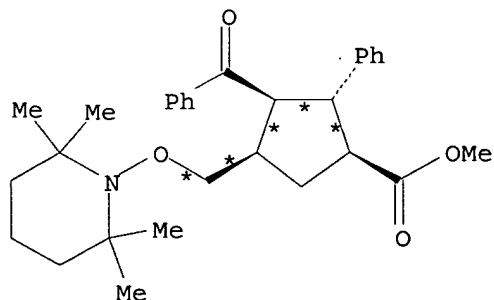


5 H

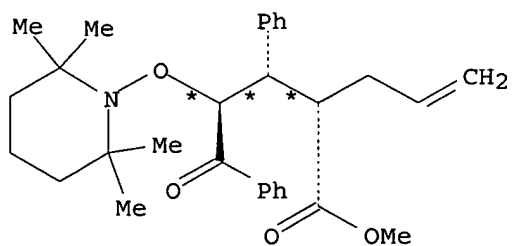


5 W

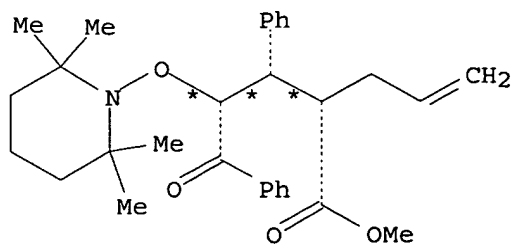
(10)



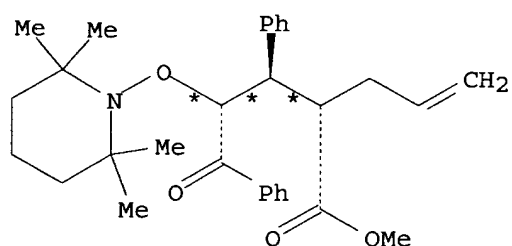
AC
YIELD 53% (88)



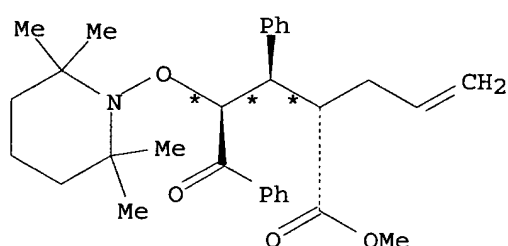
AD



AE



AF



AG

RX(10) RCT A 377752-09-5

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT H 94-41-7

STAGE(3)

RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF₆

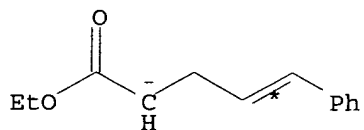
STAGE(4)

RGT F 7732-18-5 Water

PRO AC 377752-31-3, AD 377752-27-7, AE 377752-28-8, AF
377752-29-9, AG 377752-30-2

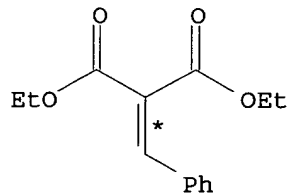
NTE isomeric methyl 2-allyl-5-oxo-3,5-diphenyl-4-(2,2,6,6-tetramethylpiperidin-1-yloxy)pentanoates 25% overall yield

RX(11) OF 17 2 K + 2 B + 2 W ==> AH +
AI

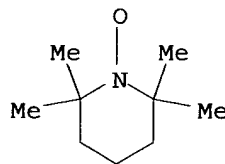


● Li⁺

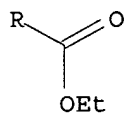
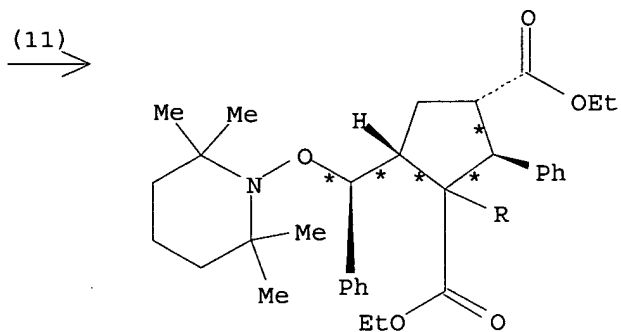
2 K



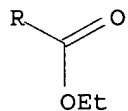
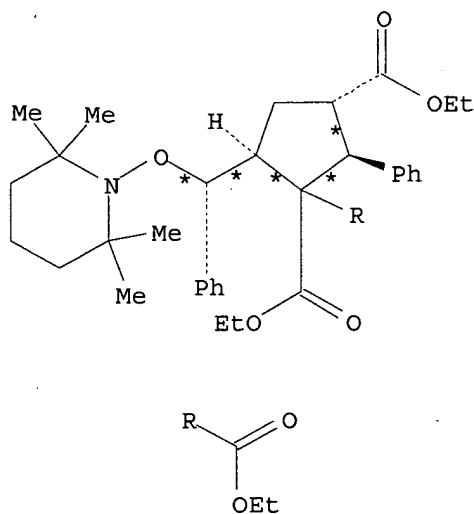
2 B



2 W



AH
YIELD 87% (53)



AI
YIELD 87% (37)

RX(11) RCT K 377752-10-8

STAGE(1)

RCT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT W 2564-83-2

RGT AA 11077-24-0 Ferrocenium PF6

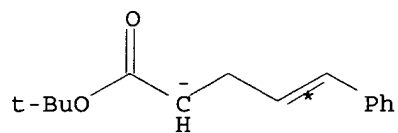
STAGE(4)

RGT F 7732-18-5 Water

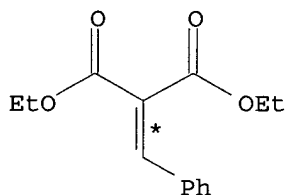
PRO AH 377752-32-4, AI 377752-33-5

NTE other products also detected

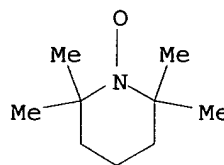
RX(12) OF 17 2 AJ + 2 B + 2 W ==> AK +
AL

● Li⁺

2 AJ

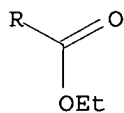
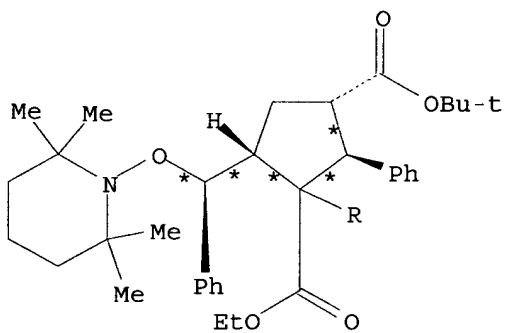


2 B

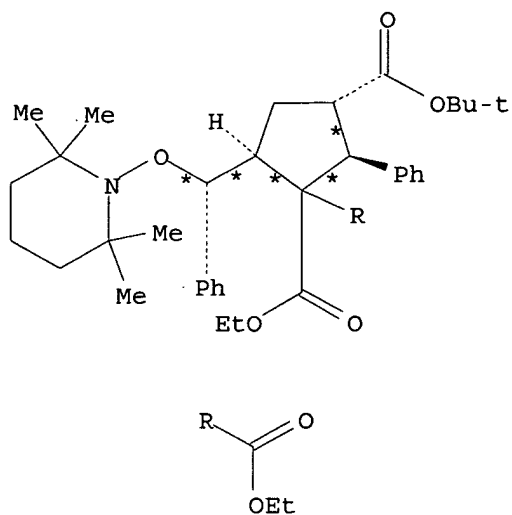


2 W

(12) →



AK
YIELD 86% (67)



AL
YIELD 29%

RX(12) RCT AJ 377752-11-9

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

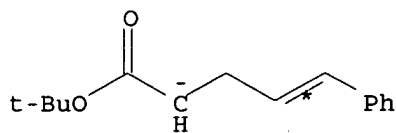
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF₆

STAGE(4)

RGT F 7732-18-5 Water

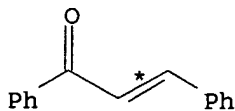
PRO AK 377752-34-6, AL 377752-35-7
NTE other products also detected

RX(13) OF 17 5 AJ + 5 H + 5 W ==> AM + AN + AO + AP + AQ

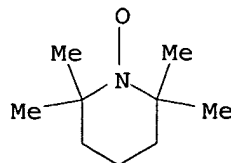


● Li⁺

5 AJ

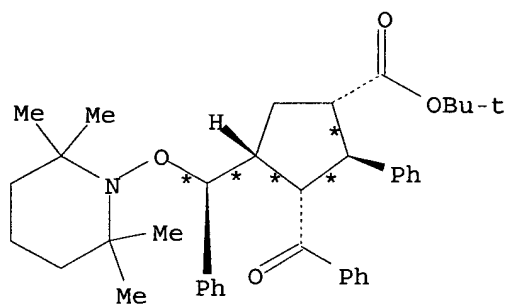


5 H

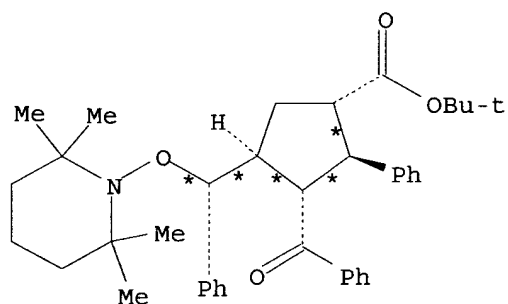


5 W

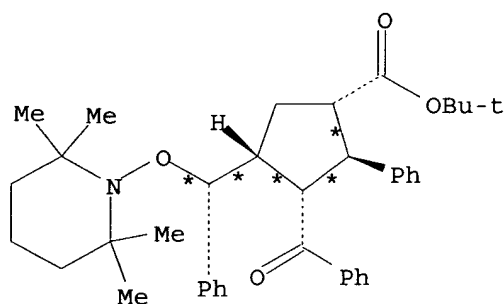
(13) 



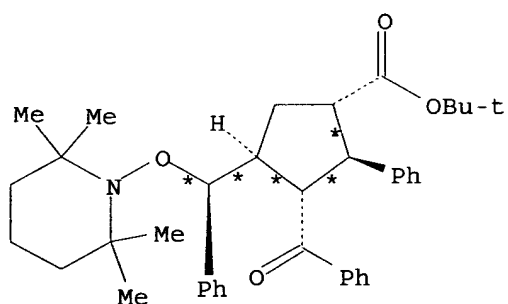
AM
YIELD 61% (68)



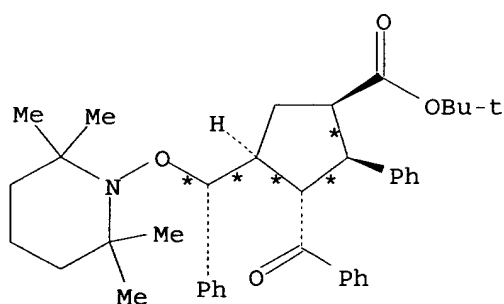
AN
YIELD 67% (13)



AO
YIELD 61% (13)



AP
YIELD 67% (6)



AQ
YIELD 1%

RX (13) RCT AJ 377752-11-9

STAGE (1)

RGT Y 75-31-0 i -PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT

SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT H 94-41-7

STAGE(3)

RCT W 2564-83-2

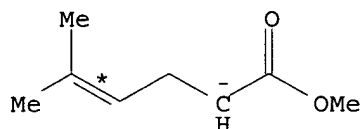
RGT AA 11077-24-0 Ferrocenium PF6

STAGE(4)

RGT F 7732-18-5 Water

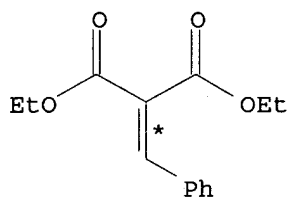
PRO AM 377752-36-8, AN 377752-38-0, AO 377752-37-9, AP 377752-39-1, AQ 377752-40-4

RX(14) OF 17 N + B + W ==> AR

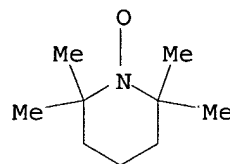


● Li⁺

N

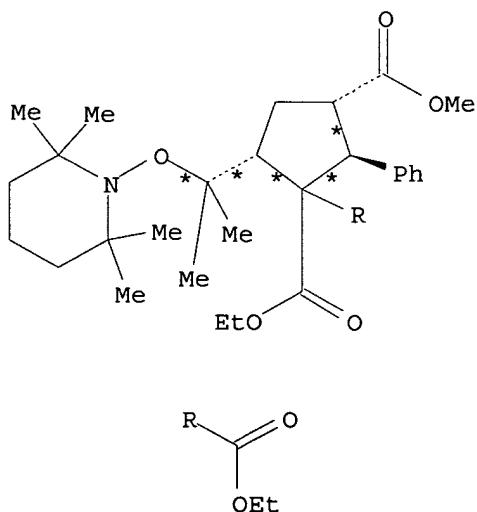


B



W

(14) →



AR
YIELD 82% (64)

RX(14) RCT N 377752-12-0

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
 SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT W 2564-83-2

RGT AA 11077-24-0 Ferrocenium PF₆

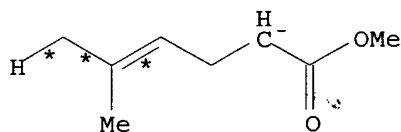
STAGE(4)

RGT F 7732-18-5 Water

PRO AR 377752-41-5

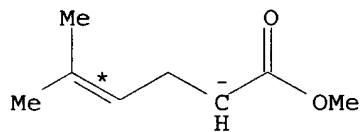
NTE other product also detected

RX(15) OF 17 6 N + 6 B + AA ==>
 AS + AT + AU + AV + AW + AX



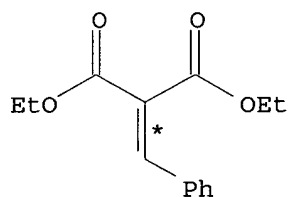
● Li⁺

2 N

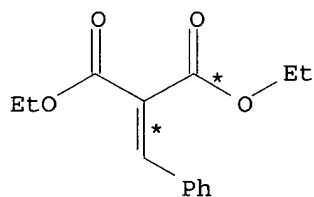


● Li⁺

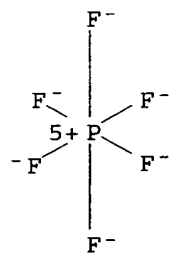
4 N



5 B



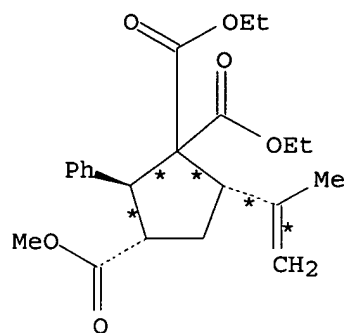
B



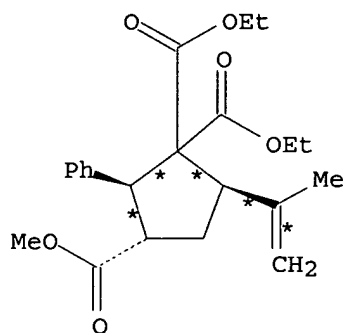
AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

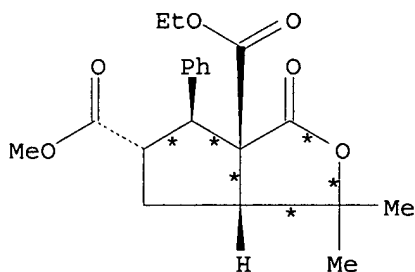
(15)
→



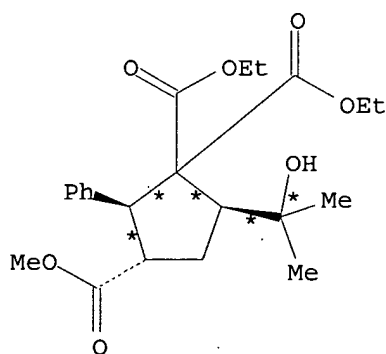
AS
YIELD 51% (75)



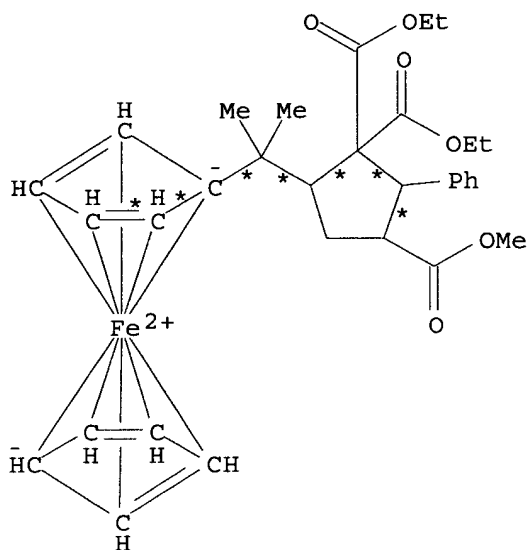
AT
YIELD 51% (25)



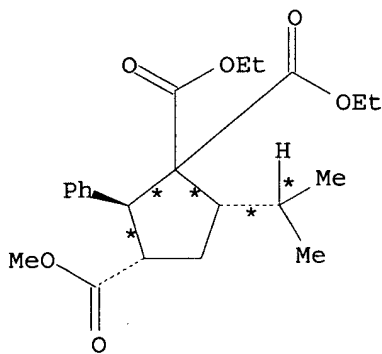
AU
YIELD 9%



AV
YIELD 5%



AW
YIELD 10% (67)



AX
YIELD 2%

RX(15) RCT N 377752-12-0

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT AA 11077-24-0

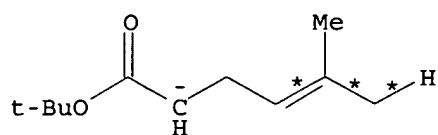
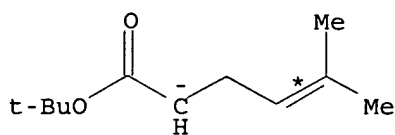
STAGE(4)

RGT F 7732-18-5 Water

PRO AS 377752-43-7, AT 377752-44-8, AU
377752-47-1, AV 377752-46-0, AW 379738-76-8, AX
377752-45-9

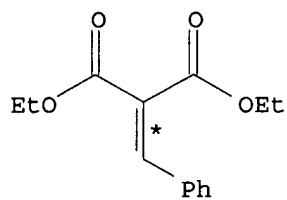
NTE other product also detected

RX(16) OF 17 6 Q + 6 B + 2 AA ==>
AY + AZ + BA + BB + BC + BD

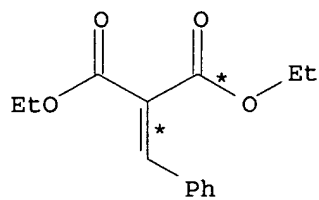
● Li⁺● Li⁺

Q

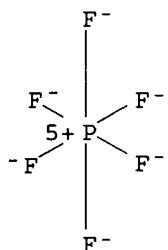
5 Q



4 B



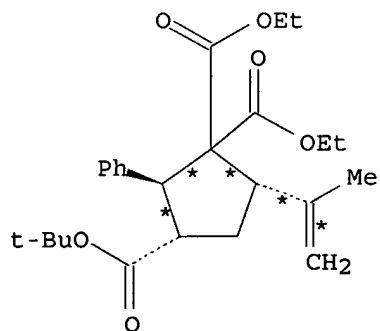
2 B



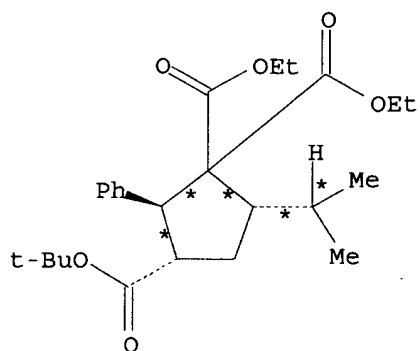
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

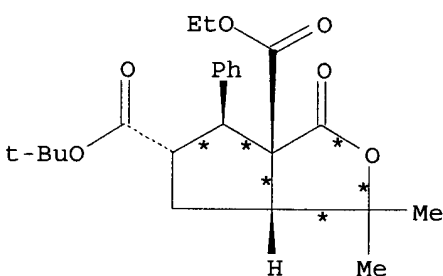
(16)



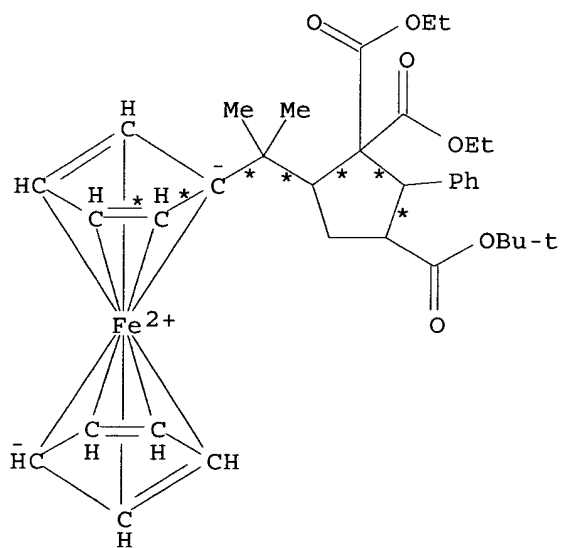
AY
YIELD 54% (94)



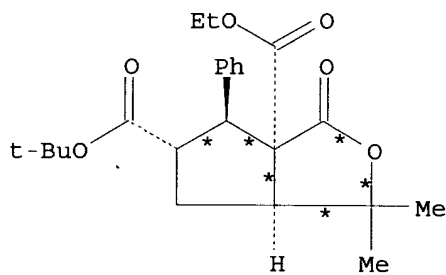
AZ
YIELD 12%



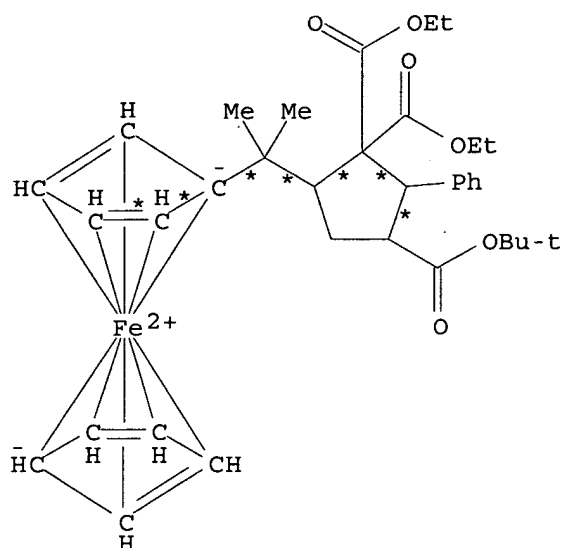
BA
YIELD 11% (75)



BB
YIELD 8% (74)



BC
YIELD 11% (25)



BD
YIELD 8% (26)

RX(16) RCT Q 377752-13-1

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT AA 11077-24-0
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

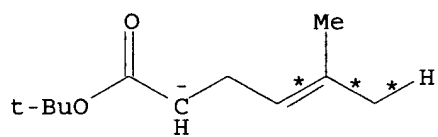
STAGE(4)

RGT F 7732-18-5 Water

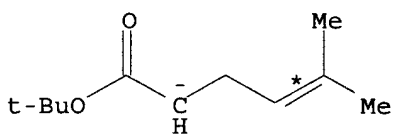
PRO AY 377752-48-2, AZ 377752-49-3, BA
377752-50-6, BB 379738-77-9, BC 377752-51-7, BD
380153-16-2

NTE other product also detected

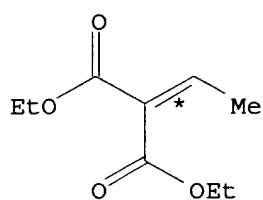
RX(17) OF 17 11 Q + 11 T + 2 AA ==>
BF + BG + BH + BI + BJ + BK + BL + BM
+ BN + BO + BP

● Li⁺

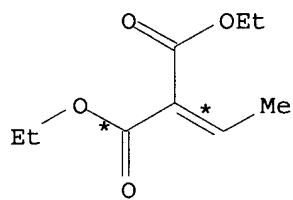
4 Q

● Li⁺

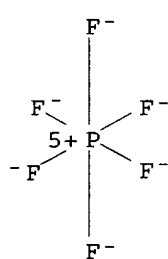
7 Q



7 T



4 T

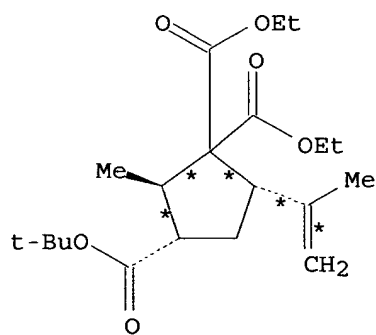
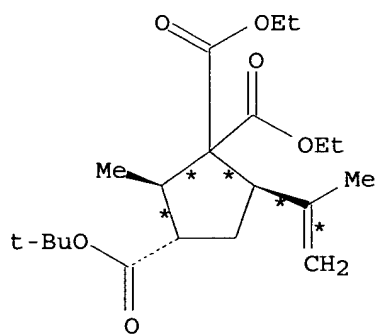


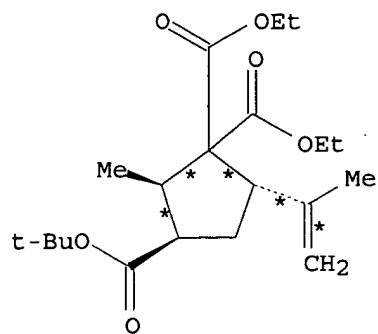
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

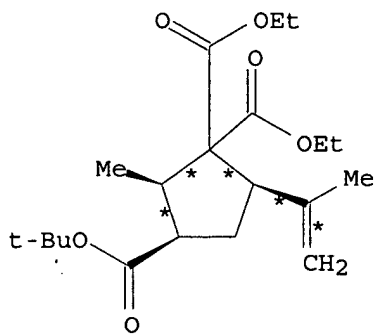
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(17) →

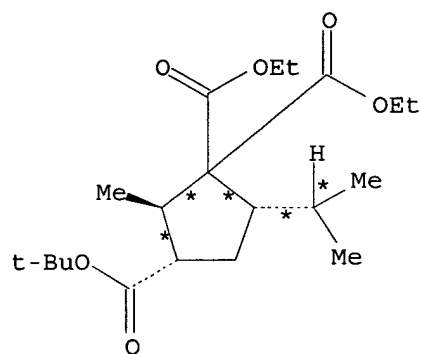
BF
YIELD 54% (71)BG
YIELD 54% (18)



BH
YIELD 54% (8)



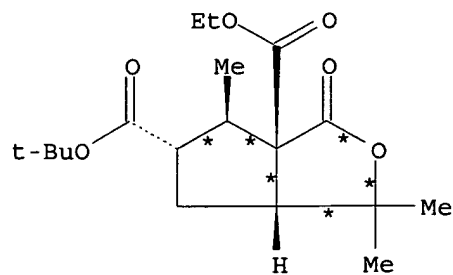
BI
YIELD 54% (3)



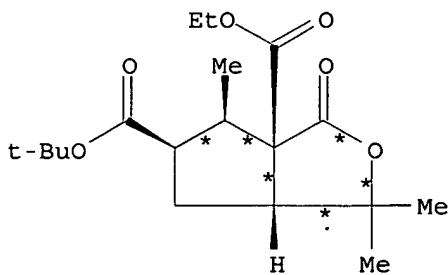
BJ
YIELD 3%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

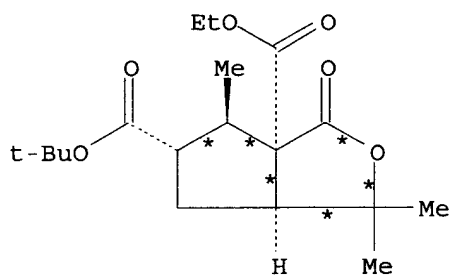
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*



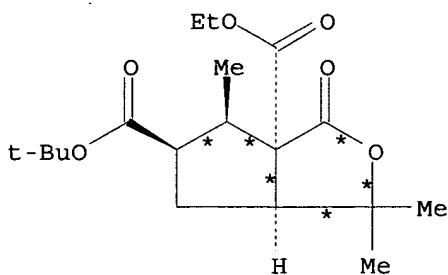
BM



BN



BO



BP

RX(17) RCT Q 377752-13-1

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
 SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT T 1462-12-0

STAGE(3)

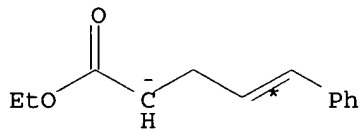
RCT AA 11077-24-0
 RGT BE 865-47-4 t-BuOK
 SOL 109-99-9 THF

STAGE(4)

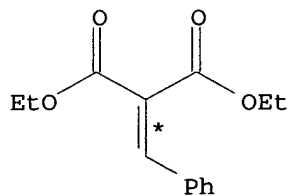
RGT F 7732-18-5 Water

PRO BF 377752-52-8, BG 377752-53-9, BH
 377752-54-0, BI 377752-55-1, BJ 377752-56-2, BK
 380153-18-4, BL 379738-78-0, BM 377752-57-3, BN
 377752-58-4, BO 377752-59-5, BP 377752-60-8
 NTE other product also detected

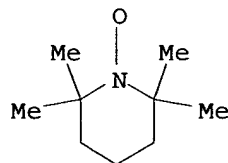
RX(11) OF 17 2 K + 2 B + 2 W ==> AH +
 AI



2 K

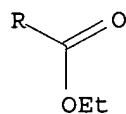
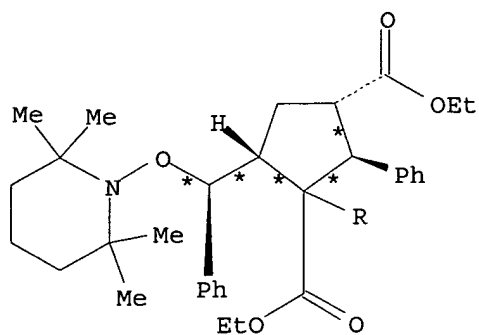


2 B

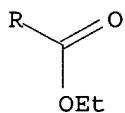
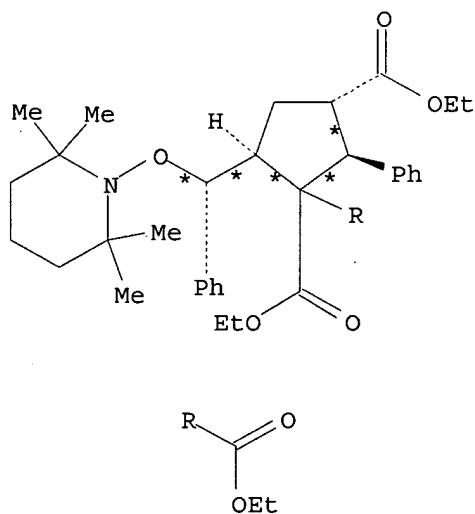


2 W

(11)



AH
YIELD 87% (53)



AI
YIELD 87% (37)

RX(11) RCT K 377752-10-8

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

RCT W 2564-83-2

RGT AA 11077-24-0 Ferrocenium PF6

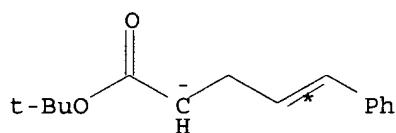
STAGE(4)

RGT F 7732-18-5 Water

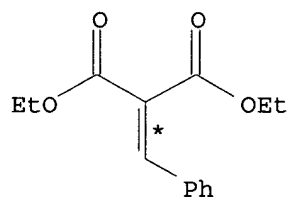
PRO AH 377752-32-4, AI 377752-33-5

NTE other products also detected

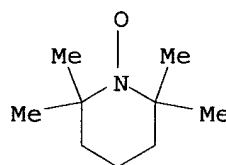
RX(12) OF 17 2 AJ + 2 B + 2 W ==> AK +
AL

● Li⁺

2 AJ

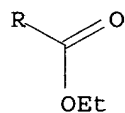
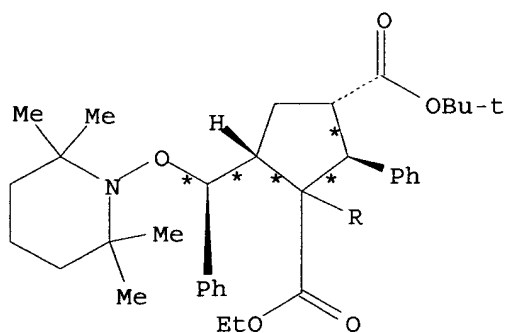


2 B

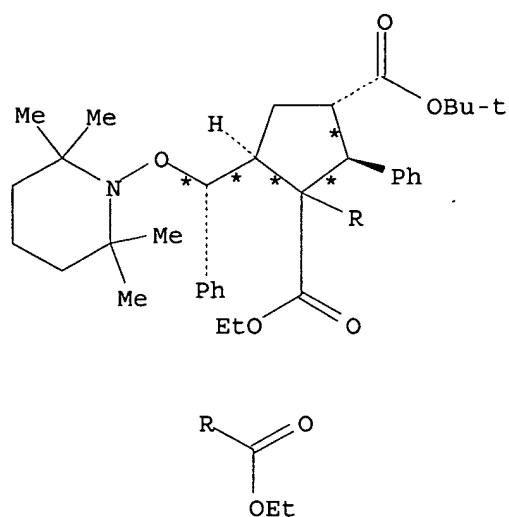


2 W

(12) →



AK
YIELD 86% (67)



AL
YIELD 29%

RX(12) RCT AJ 377752-11-9

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

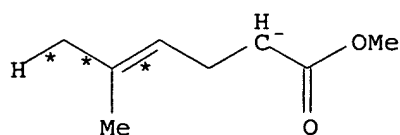
RCT W 2564-83-2
RGT AA 11077-24-0 Ferrocenium PF₆

STAGE(4)

RGT F 7732-18-5 Water

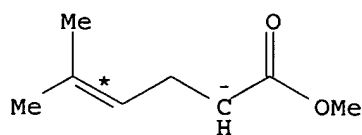
PRO AK 377752-34-6, AL 377752-35-7
NTE other products also detected

RX(15) OF 17 6 N + 6 B + AA ==>
AS + AT + AU + AV + AW + AX



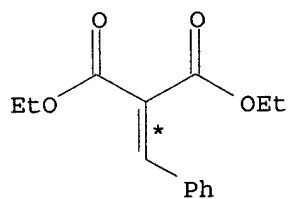
● Li⁺

2 N

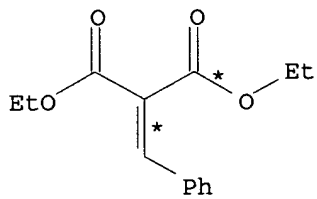


● Li⁺

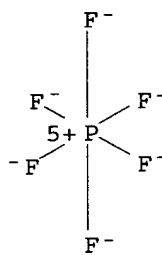
4 N



5 B



B

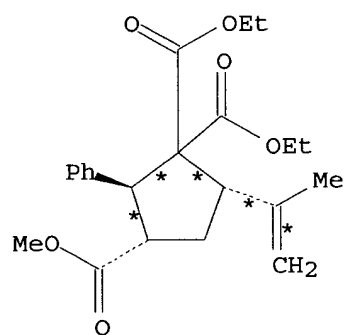


AA: CM 1

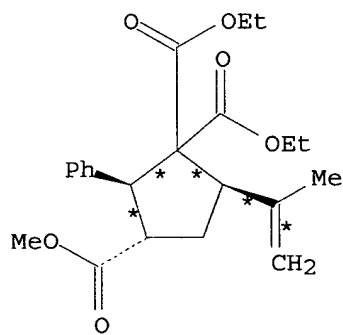
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

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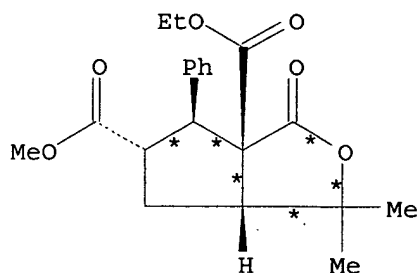
(15)



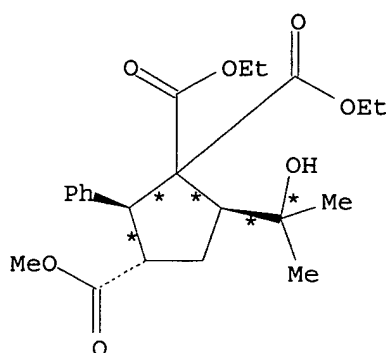
AS
YIELD 51% (75)



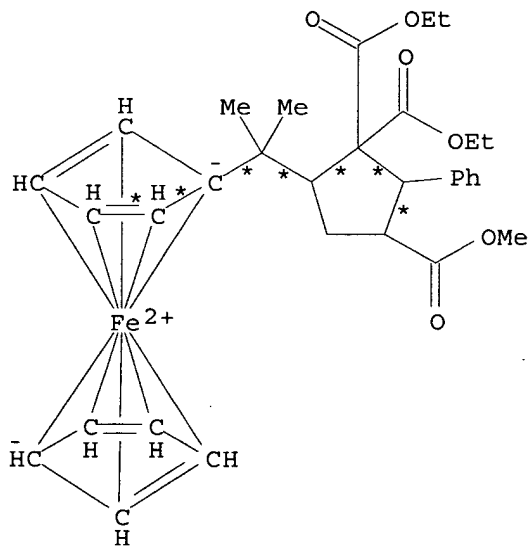
AT
YIELD 51% (25)



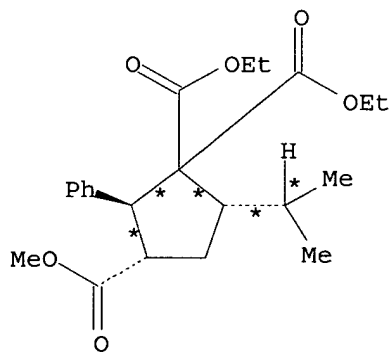
AU
YIELD 9%



AV
YIELD 5%



AW
YIELD 10% (67)



AX
YIELD 2%

RX(15) RCT N 377752-12-0

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT' B 5292-53-5

STAGE(3)

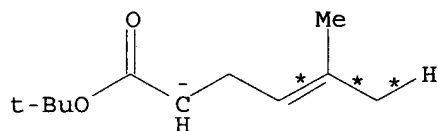
RCT AA 11077-24-0

STAGE(4)

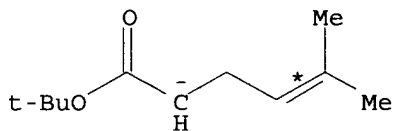
RGT F 7732-18-5 Water

PRO AS 377752-43-7, AT 377752-44-8, AU
 377752-47-1, AV 377752-46-0, AW 379738-76-8, AX
 377752-45-9
 NTE other product also detected

RX(16) OF 17 6 Q + 6 B + 2 AA ==>
 AY + AZ + BA + BB + BC + BD



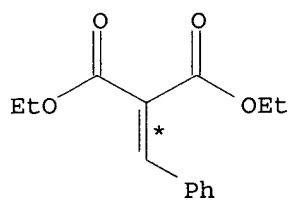
● Li⁺



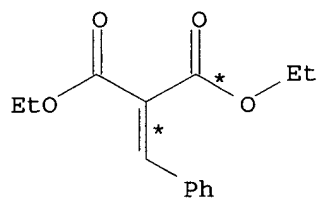
● Li⁺

Q

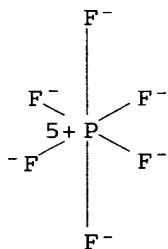
5 Q



4 B



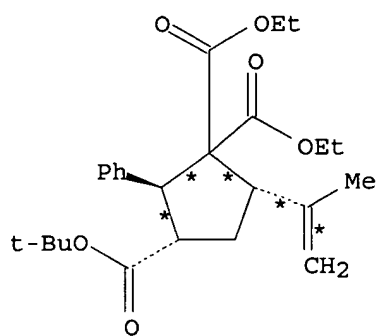
2 B



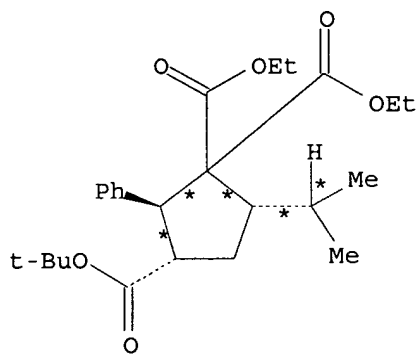
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
 *

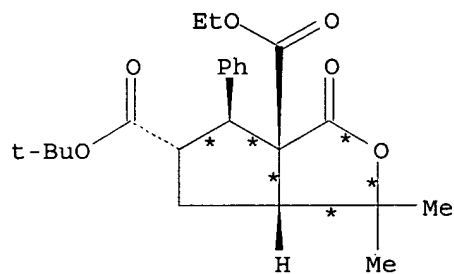
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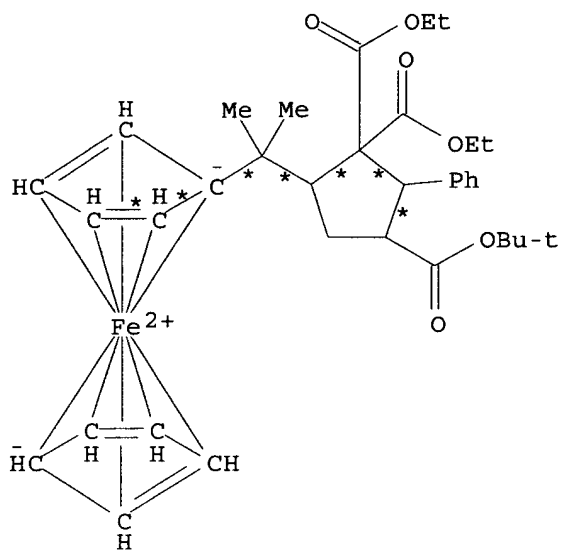
AY
YIELD 54% (94)



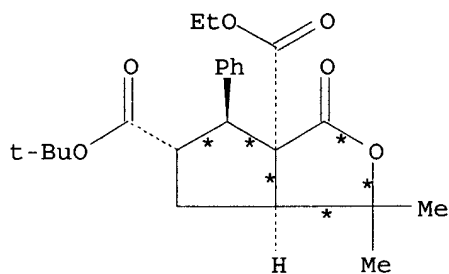
AZ
YIELD 12%



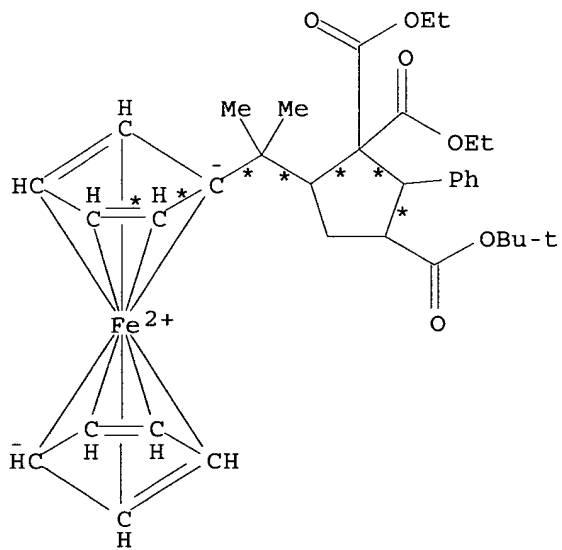
BA
YIELD 11% (75)



BB
YIELD 8% (74)



BC
YIELD 11% (25)



BD
YIELD 8% (26)

RX(16) RCT Q 377752-13-1

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT B 5292-53-5

STAGE(3)

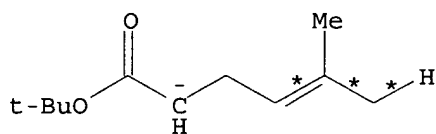
RCT AA 11077-24-0
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

STAGE(4)

RGT F 7732-18-5 Water

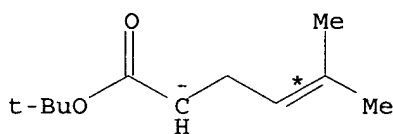
PRO AY 377752-48-2, AZ 377752-49-3, BA
377752-50-6, BB 379738-77-9, BC 377752-51-7, BD
380153-16-2
NTE other product also detected

RX(17) OF 17 11 Q + 11 T + 2 AA ==>
BF + BG + BH + BI + BJ + BK + BL + BM
+ BN + BO + BP



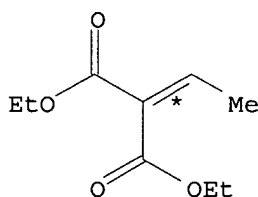
● Li⁺

4 Q

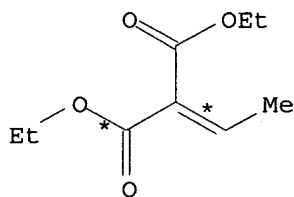


● Li⁺

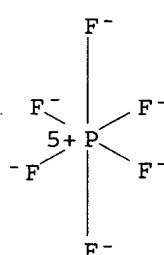
7 Q



7 T



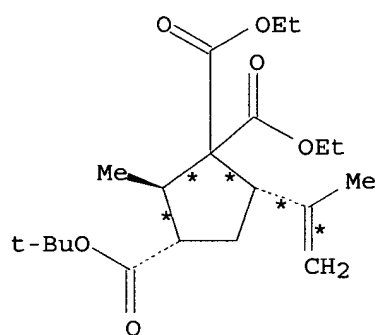
4 T



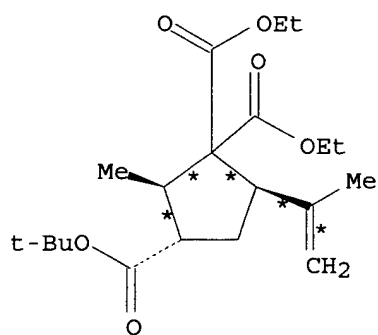
2 AA: CM 1

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

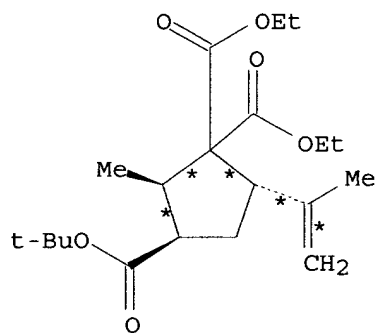
(17)
→



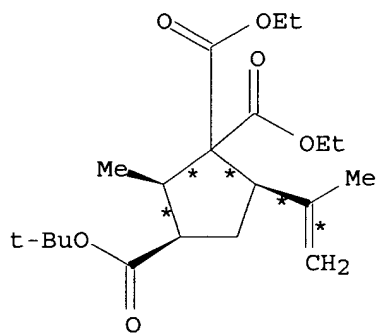
BF
YIELD 54% (71)



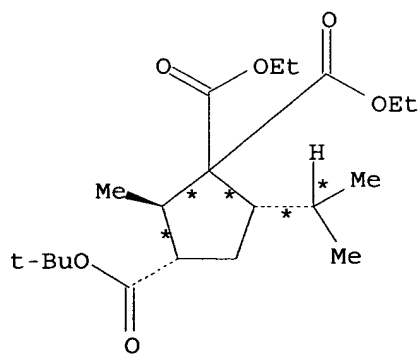
BG
YIELD 54% (18)



BH
YIELD 54% (8)



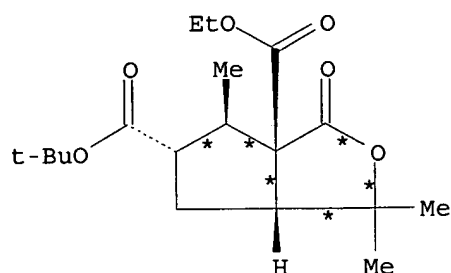
BI
YIELD 54% (3)



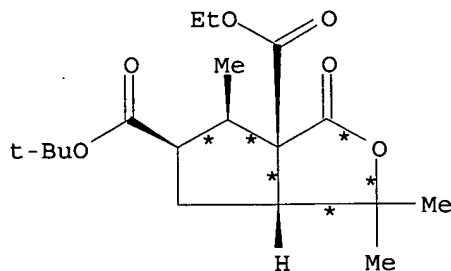
BJ
YIELD 3%

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

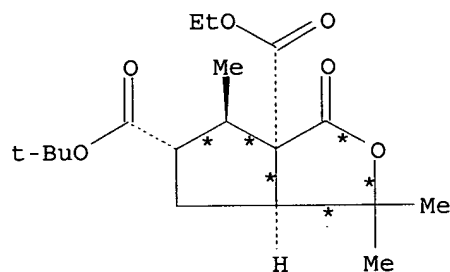
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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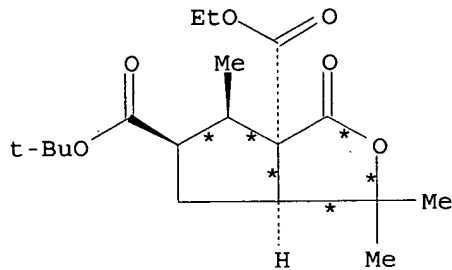
BM



BN



BO



BP

RX(17) RCT Q 377752-13-1

STAGE(1)

RGT Y 75-31-0 i-PrNH₂, Z 109-72-8 BuLi, E 680-31-9 HMPT
SOL 109-99-9 THF, 110-54-3 Hexane

STAGE(2)

RCT T 1462-12-0

STAGE(3)

RCT AA 11077-24-0
RGT BE 865-47-4 t-BuOK
SOL 109-99-9 THF

STAGE(4)

RGT F 7732-18-5 Water

PRO BF 377752-52-8, BG 377752-53-9, BH
377752-54-0, BI 377752-55-1, BJ 377752-56-2, BK
380153-18-4, BL 379738-78-0, BM 377752-57-3, BN
377752-58-4, BO 377752-59-5, BP 377752-60-8
NTE other product also detected

ACCESSION NUMBER: 134:237626 CASREACT
TITLE: Carbon-carbon bond forming reactions of
N-bound transition metal α -
cyanocarbanions: a mechanistic probe for
catalytic Michael reactions of nitriles
AUTHOR(S): Naota, Takeshi; Tannna, Akio; Murahashi,
Shun-Ichi
CORPORATE SOURCE: Department of Chemistry, Graduate School of
Engineering Science, Osaka University,
Machikaneyama, Toyonaka, Osaka, 560-8531,
Japan
SOURCE: Chemical Communications (Cambridge) (2001),
(1), 63-64
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English
CLASSIFICATION: 29-13 (Organometallic and Organometalloidal
Compounds)
Section cross-reference(s): 22
ABSTRACT:
N-Bound α -cyanocarbanion complexes Ru+Cp(NCCH-R1)(PPh₃)₂ 1 react
with electron deficient olefins to afford the conjugate adduct
Ru+Cp(NCC-R1CHR₂CR₃R₄)(PPh₃)₂ 2, kinetic studies of which revealed that
complex 1-catalyzed Michael reactions of nitriles proceed via
transformation of 1 to 2 and subsequent ligand exchange with nitriles.
SUPPL. TERM: ruthenium catalyst Michael reaction nitrile alkene;
carbon carbon bond formation ruthenium
cyanocarbanion catalyst
INDEX TERM: Addition reaction kinetics
(Michael reaction kinetics; of ruthenium
cyanocarbanion catalyzed Michael reaction of
alkenes with nitriles)
INDEX TERM: Michael reaction
(kinetics; of ruthenium cyanocarbanion catalyzed
Michael reaction of alkenes with nitriles)
INDEX TERM: Reaction mechanism
(of ruthenium cyanocarbanion catalyzed Michael
reaction of alkenes with nitriles)
INDEX TERM: Alkenes, reactions
Nitriles, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(ruthenium cyanocarbanion catalyzed Michael
reaction of alkenes with nitriles)
INDEX TERM: Michael reaction catalysts
(ruthenium cyanocarbanion; for Michael addition of
nitriles with olefins)
INDEX TERM: Carbanions
ROLE: CAT (Catalyst use); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(ruthenium cyanocarbanions; conjugate addition
reaction with electron deficient olefins)
INDEX TERM: 6626-84-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Michael reaction with ruthenium carbanions)
INDEX TERM: 7605-28-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conjugate addition of ruthenium carbanions)

INDEX TERM: 17041-60-0, Dimethyl ethylidenemalonate
293767-54-1 330598-53-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conjugate addition to olefins)

INDEX TERM: 264130-83-8
ROLE: CAT (Catalyst use); RCT (Reactant); RACT
(Reactant or reagent); USES (Uses)
(conjugate addition to olefins, and catalyst for
Michael reactions of nitriles)

INDEX TERM: 330598-57-7P
ROLE: CAT (Catalyst use); SPN (Synthetic
preparation); PREP (Preparation); USES (Uses)
(preparation and catalyst for Michael reactions of
nitriles)

INDEX TERM: 623-43-8
(preparation of)

INDEX TERM: 107-13-1, Acrylonitrile, reactions 625-33-2,
Pent-3-en-2-one 2700-22-3,
Benzylidenemalononitrile
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(preparation of)

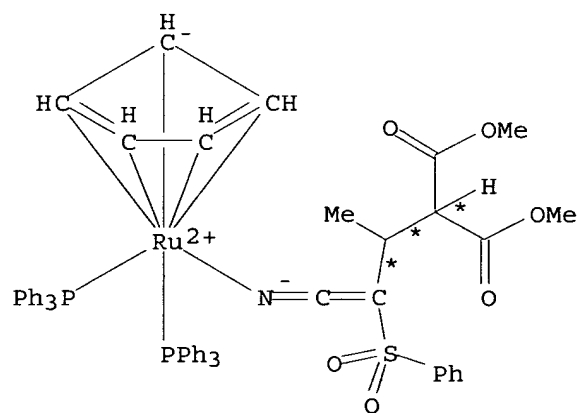
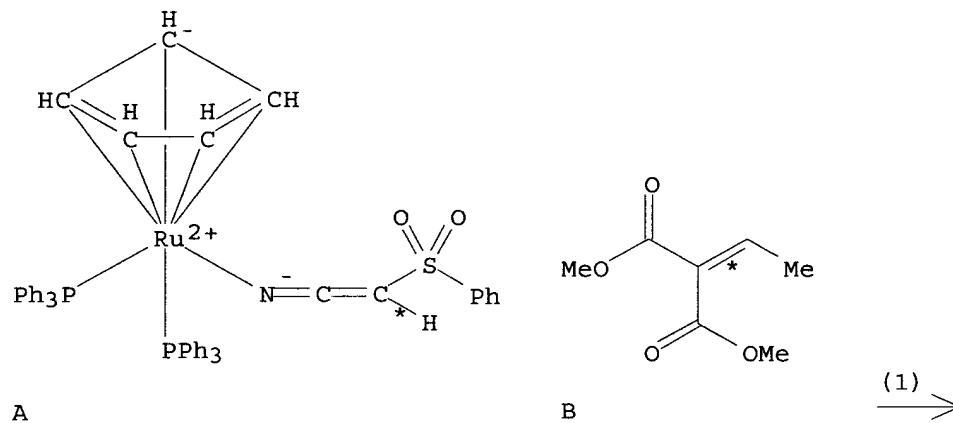
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330598-58-8P 330598-59-9P 330598-60-2P
330598-61-3P
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(preparation of)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR
THIS RECORD.

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Society of Japan 1998, Paper 3A117
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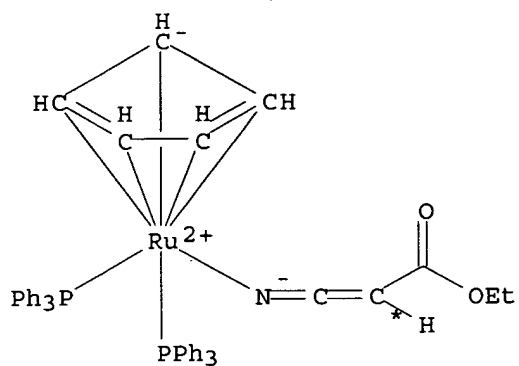
RX(1) OF 8 A + B ==> C



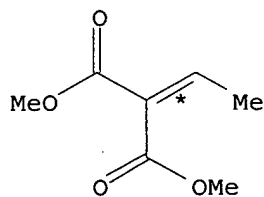
C
YIELD 99%

RX(1) RCT A 264130-83-8, B 17041-60-0
 PRO C 330598-54-4
 SOL 71-43-2 Benzene

RX(2) OF 8 E + B ==> F

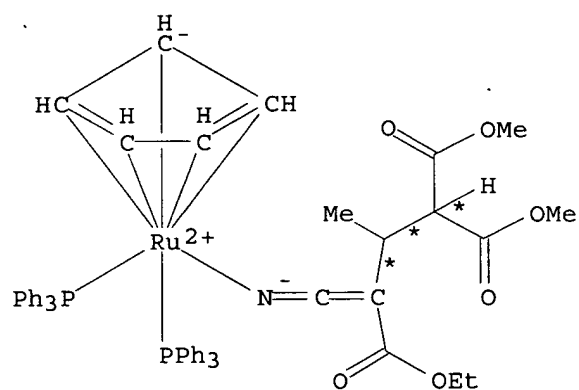


E



B

(2) →

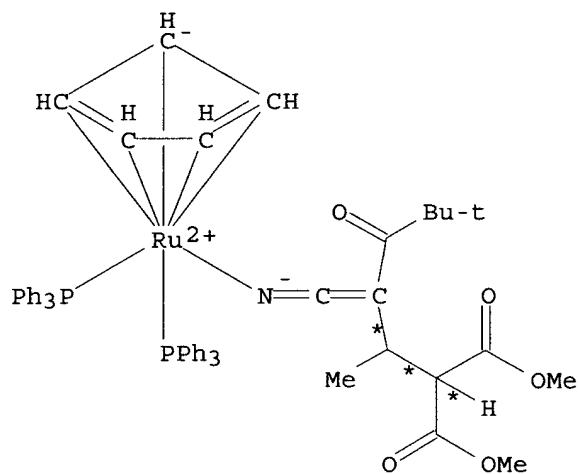
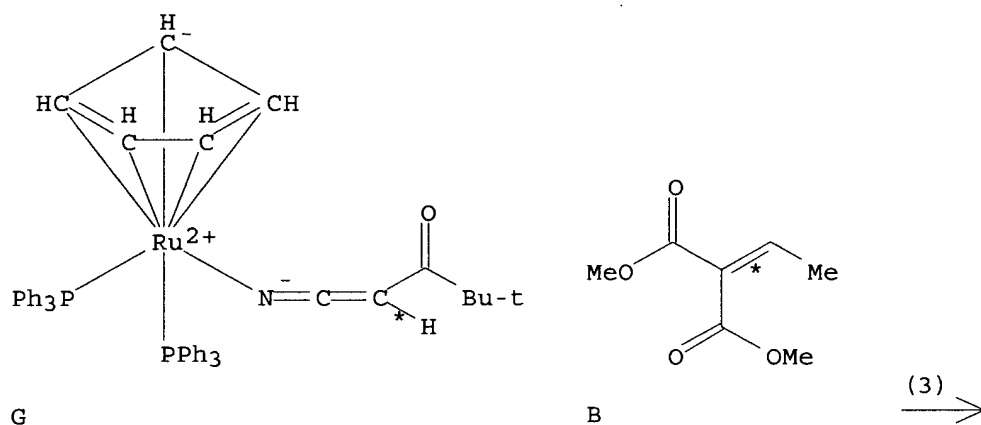


F

YIELD 98%

RX(2) RCT E 293767-54-1, B 17041-60-0
 PRO F 330598-55-5
 SOL 71-43-2 Benzene

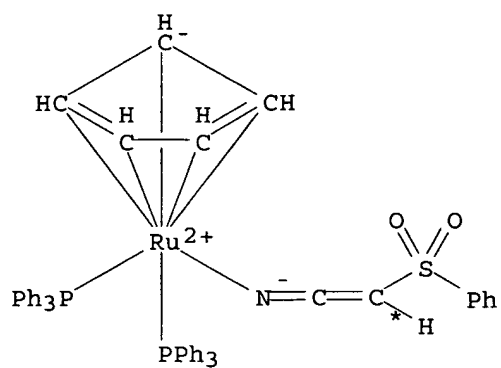
RX(3) OF 8 G + B ==> H



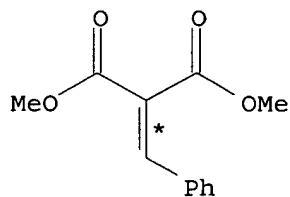
H
YIELD 98%

RX(3) RCT G 330598-53-3, B 17041-60-0
 PRO H 330598-56-6
 SOL 71-43-2 Benzene

RX(4) OF 8 A + I ==> J

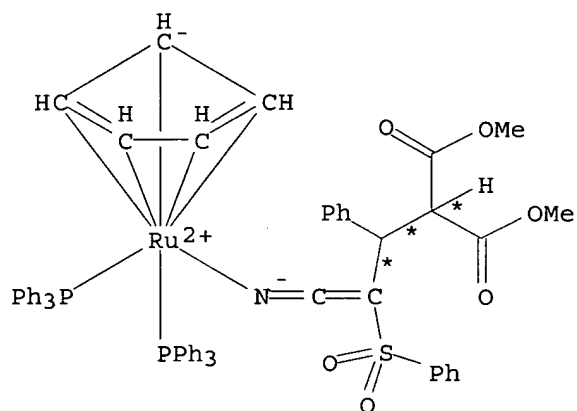


A



I

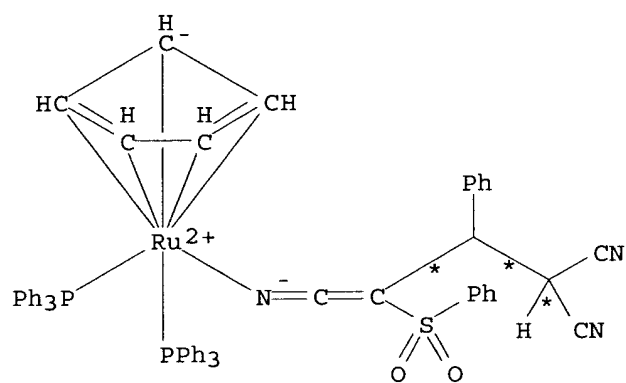
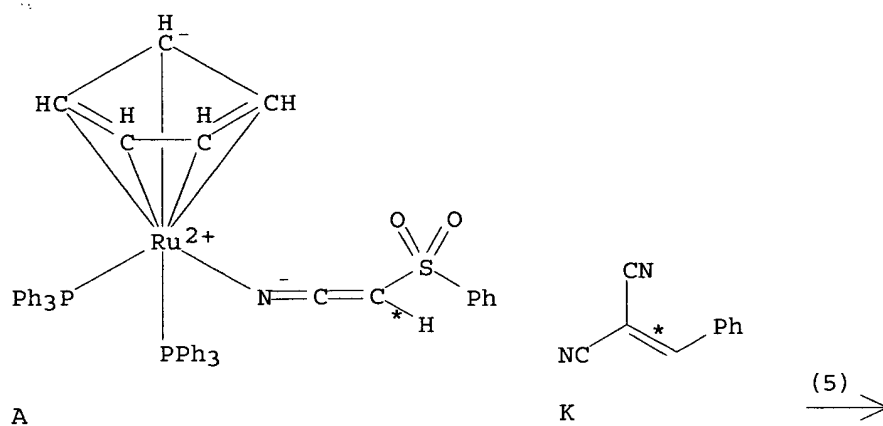
(4) →



J
YIELD 98%

RX(4) RCT A 264130-83-8, I 6626-84-2
PRO J 330598-57-7
SOL 71-43-2 Benzene

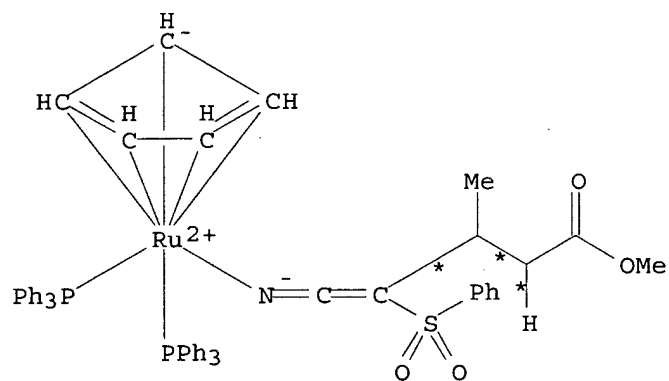
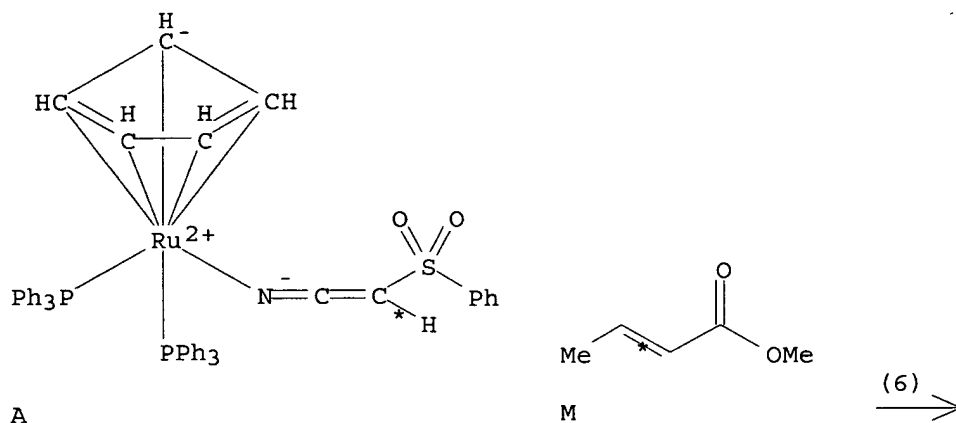
RX(5) OF 8 A + K ==> L



YIELD 99%

RX (5) RCT A 264130-83-8, K 2700-22-3
 PRO L 330598-58-8
 SOL 71-43-2 Benzene

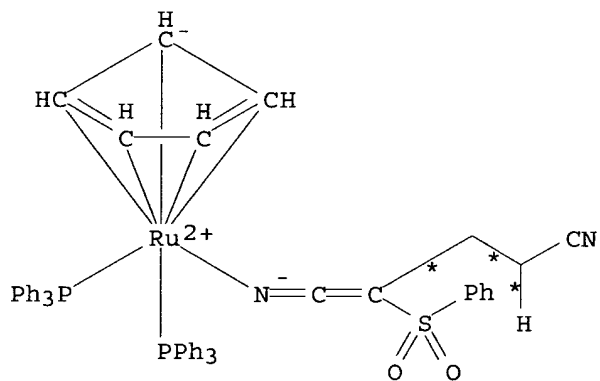
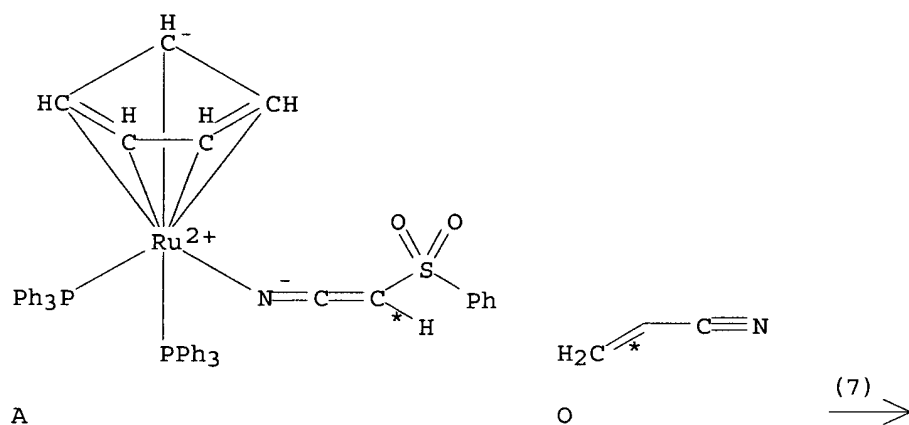
RX (6) OF 8 A + M ==> N



YIELD 31%

RX(6) RCT A 264130-83-8, M 623-43-8
 PRO N 330598-59-9
 SOL 71-43-2 Benzene

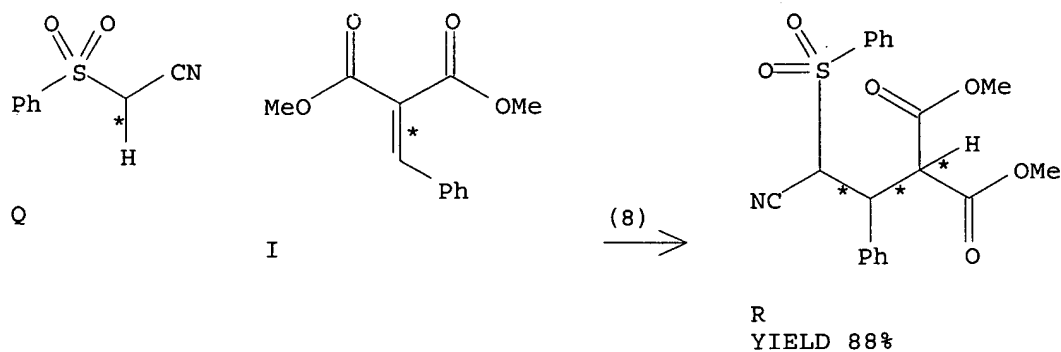
RX(7) OF 8 A + O ==> P



P
YIELD 36%

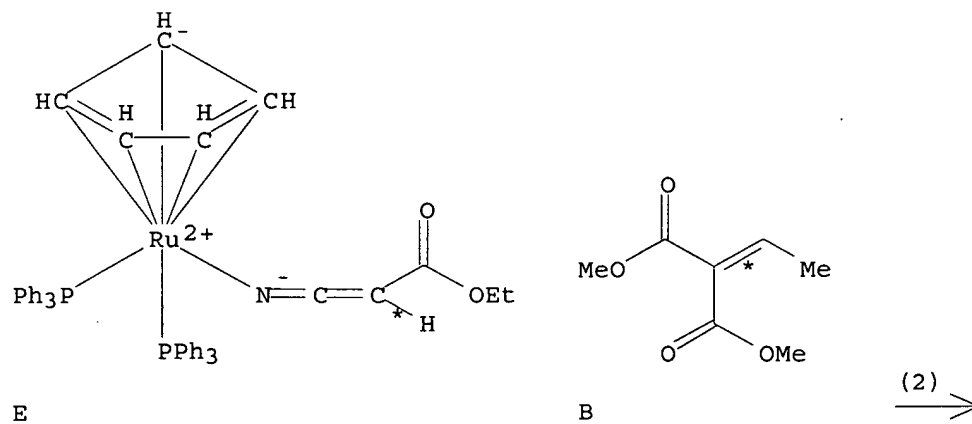
RX(7) RCT A 264130-83-8, O 107-13-1
 PRO P 330598-60-2
 SOL 71-43-2 Benzene

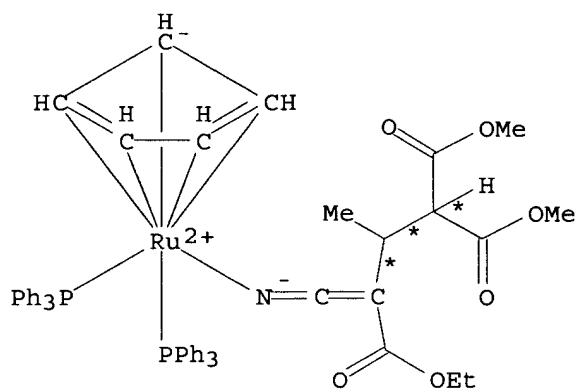
RX(8) OF 8 Q + I ==> R



RX(8) RCT Q 7605-28-9, I 6626-84-2
 PRO R 330598-61-3
 CAT 330598-57-7 Ruthenium, (η^5 -2,4-cyclopentadien-1-yl) [dimethyl [3-(imino- κ N)-1-phenyl-2-(phenylsulfonyl)-2-propenyl]propanedioato]bis(triphenylphosphine) -
 SOL 109-99-9 THF
 NTE Michael addn. reaction

RX(2) OF 8 E + B ==> F

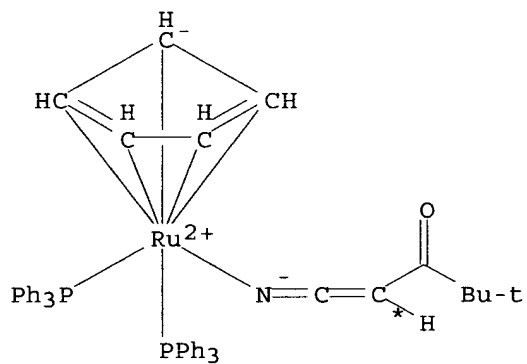




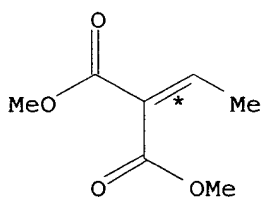
F
YIELD 98%

RX(2) RCT E 293767-54-1, B 17041-60-0
PRO F 330598-55-5
SOL 71-43-2 Benzene

RX(3) OF 8 G + B ==> H

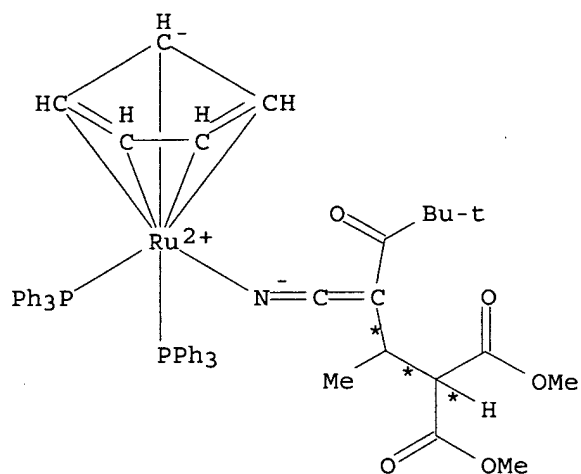


G



B

(3) →



H
YIELD 98%

RX(3) RCT G 330598-53-3, B 17041-60-0
PRO H 330598-56-6
SOL 71-43-2 Benzene

L20 ANSWER 3 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 129:175347 CASREACT

TITLE: Michael reactions promoted by
η¹-O-enolatoruthenium(II) complexes
derived from Ru(cod)(cot), diphosphine, and
dimethyl malonate

AUTHOR(S): Alvarez, Salvador G.; Hasegawa, Sachi; Hirano,
Masafumi; Komiya, Sanshiro

CORPORATE SOURCE: Department of Applied Chemistry, Faculty of
Technology, Tokyo University of Agriculture
and Technology, Tokyo, 184-8588, Japan

SOURCE: Tetrahedron Letters (1998), 39(29), 5209-5212
CODEN: TELEAY; ISSN: 0040-4039

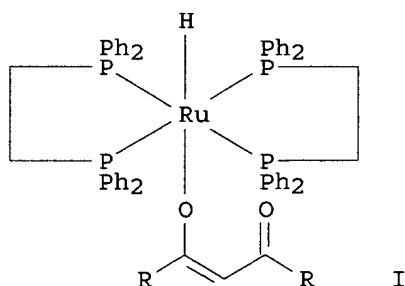
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 23-17 (Aliphatic Compounds)
Section cross-reference(s): 29

GRAPHIC IMAGE:



ABSTRACT:

The Michael reaction of 1,3-dicarbonyls with α,β -unsatd. esters and nitriles has been carried out very efficiently, under mild and neutral conditions, in the presence of a catalytic amount of trans-hydrido(η^1 -O-enolato) ruthenium(II) complex I. I is prepared from the reaction of $\text{Ru}(\text{cod})(\text{cot})$ (cod = cycloocta-1,5-diene; cot = cycloocta-1,3,5-triene) with di-Me malonate in the presence of $\text{Ph}_2\text{P}(\text{CH}_2)_2\text{PPh}_2$ (dpe). I catalyzes the Michael reaction of Me acrylate with a 1:1 mixture of di-Me malonate and acetylacetone to give the double Michael adduct of Me acrylate with acetylacetone exclusively in 67% yield; NaOMe in THF provides the double Michael adducts of acetylacetone and di-Me malonate, resp., in a 28:72 ratio, while PEt_3 gives the adducts in a ratio of 86:14.

SUPPL. TERM: ruthenium enolato hydride complex catalyst prepn;
heptanedioate methoxycarbonyl prepn; acetyl
heptanedioate prepn; methoxycarbonyl
heptanedinitrile prepn; heptanedinitrile diacetyl
prepn; Michael addn reaction catalyst acrylate
acrylonitrile; acetylacetone malonate Michael addn
catalyst; enolato ruthenium complex catalyst Michael
addn; selective Michael addn catalyst proton acidity

INDEX TERM: Chemoselectivity
Michael reaction
Michael reaction catalysts
(η^1 -enolato ruthenium(2+) complexes as
catalysts for the double Michael addition of
acetylacetone and di-Me malonate to Me acrylate
and acrylonitrile)

INDEX TERM: 211634-64-9P
ROLE: CAT (Catalyst use); RCT (Reactant); SPN
(Synthetic preparation); PREP (Preparation); RACT
(Reactant or reagent); USES (Uses)
(η^1 -enolato ruthenium(2+) complexes as
catalysts for the double Michael addition of
acetylacetone and di-Me malonate to Me acrylate
and acrylonitrile)

INDEX TERM: 211634-66-1P
ROLE: CAT (Catalyst use); SPN (Synthetic
preparation); PREP (Preparation); USES (Uses)
(η^1 -enolato ruthenium(2+) complexes as
catalysts for the double Michael addition of
acetylacetone and di-Me malonate to Me acrylate
and acrylonitrile)

INDEX TERM: 96-33-3 107-13-1, 2-Propenenitrile, reactions
108-59-8, Dimethyl malonate 123-54-6,

2,4-Pentanedione, reactions 1663-45-2,
1,2-Bis(diphenylphosphino)ethane 42516-72-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(η^1 -enolato ruthenium(2+) complexes as
catalysts for the double Michael addition of
acetylacetone and di-Me malonate to Me acrylate
and acrylonitrile)

INDEX TERM:

609-02-9P 815-57-6P 5324-43-6P 13984-59-3P
19766-36-0P 22711-92-8P 211634-65-0P

ROLE: SPN (Synthetic preparation); PREP
(Preparation)

(η^1 -enolato ruthenium(2+) complexes as
catalysts for the double Michael addition of
acetylacetone and di-Me malonate to Me acrylate
and acrylonitrile)

REFERENCE COUNT:

23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR
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REFERENCE(S):

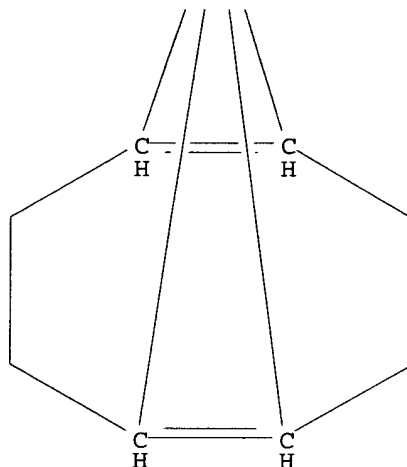
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RX(1) OF 12 A + 2 B + C ==> D...

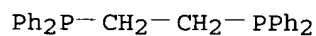
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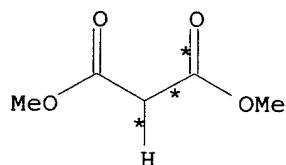
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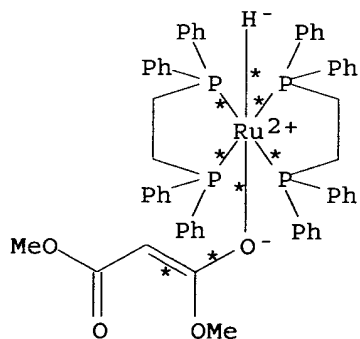
A



2 B



C



D

YIELD 21%

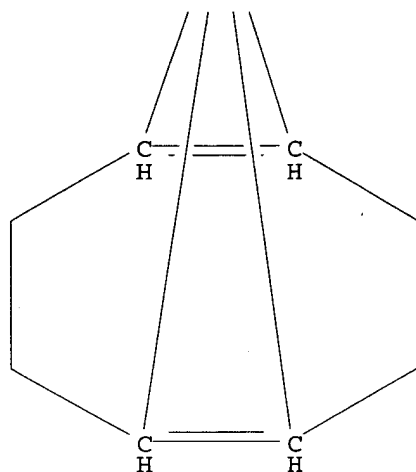
RX(1) RCT A 42516-72-3, B 1663-45-2, C 108-59-8

PRO D 211634-64-9
SOL 71-43-2 Benzene

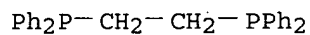
RX(2) OF 12 A + B + F ==> G

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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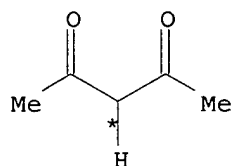
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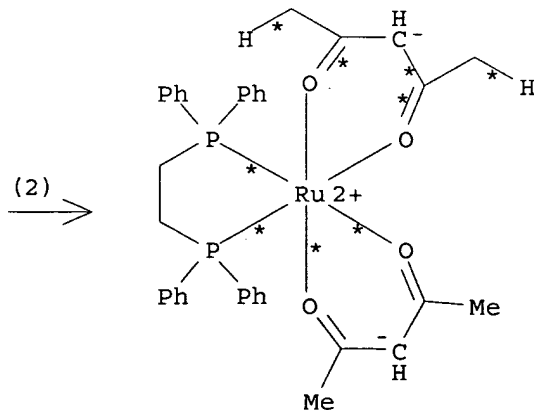
A



B



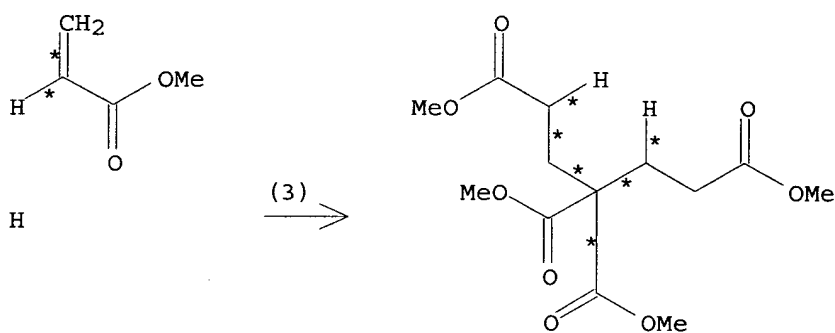
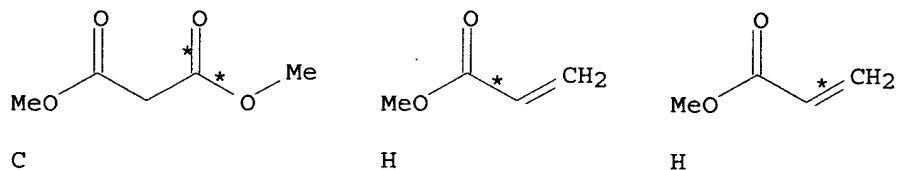
F



G
YIELD 12%

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 PRO G 211634-65-0
 SOL 71-43-2 Benzene

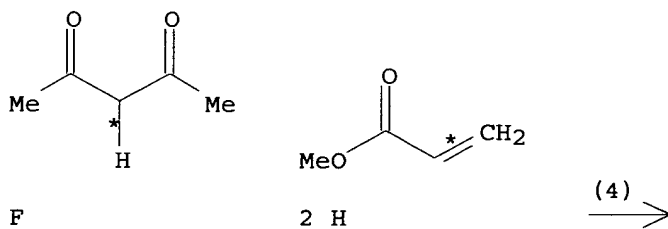
RX(3) OF 12 C + 3 H ==> I

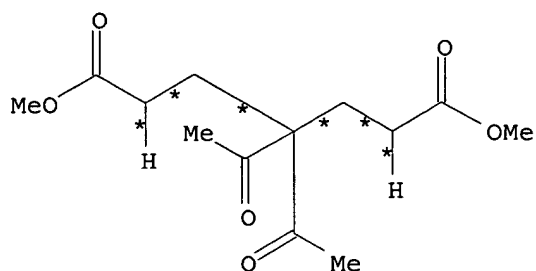


I
YIELD 89%

RX(3) RCT C 108-59-8, H 96-33-3
 PRO I 19766-36-0
 CAT 211634-66-1 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[4-(hydroxy-κO)-3-penten-2-onato]-, (OC-6-11)-
 SOL 71-43-2 Benzene
 NTE chemoselective, yield based on di-Me malonate

RX(4) OF 12 F + 2 H ==> K

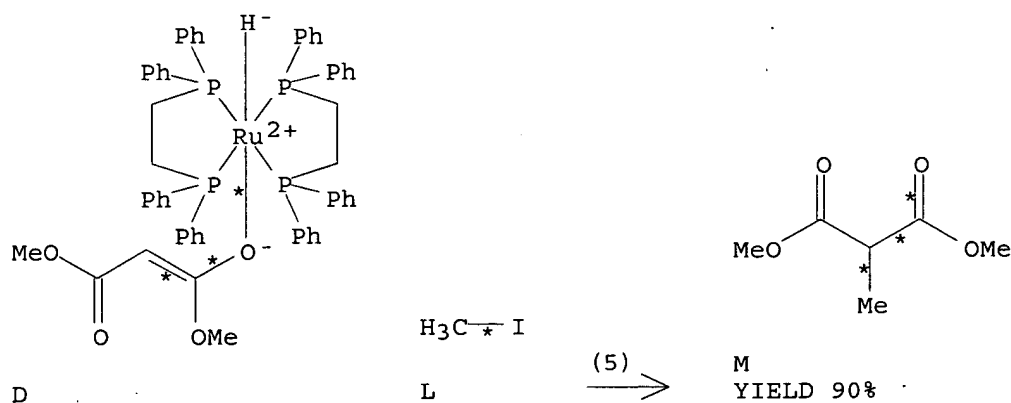




K
YIELD 62%

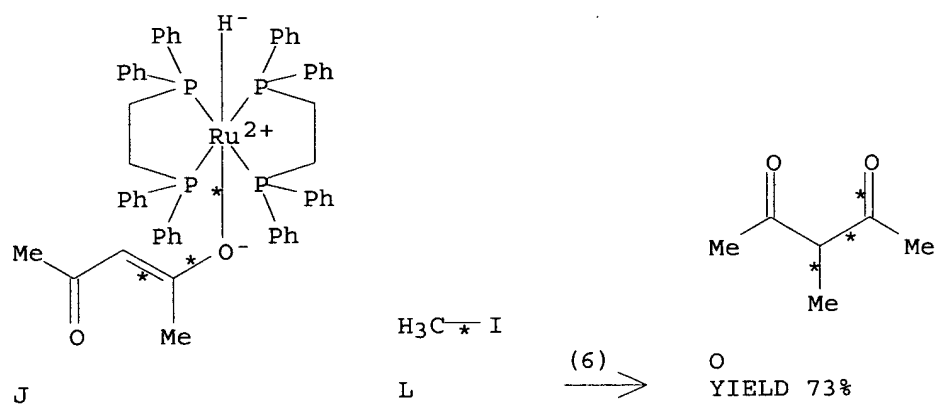
RX(4) RCT F 123-54-6, H 96-33-3
PRO K 13984-59-3
CAT 211634-66-1 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[4-(hydroxy-κO)-3-penten-2-onato]-, (OC-6-11)-
SOL 71-43-2 Benzene
NTE chemoselective, yield based on 1,3-pentanedione

RX(5) OF 12 ...D + L ==> M



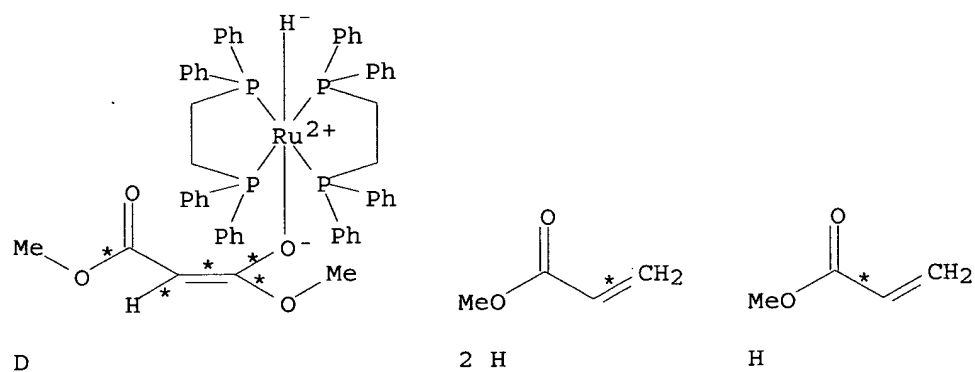
RX(5) RCT D 211634-64-9, L 74-88-4
PRO M 609-02-9
SOL 1076-43-3 C6D6

RX(6) OF 12 J + L ==> O

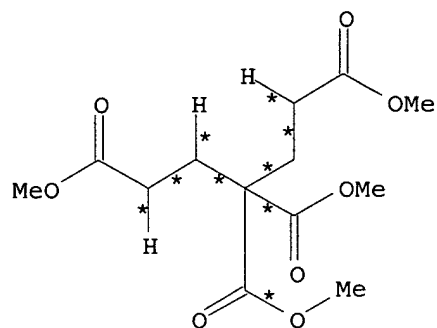


RX(6) RCT J 211634-66-1, L 74-88-4
 PRO O 815-57-6
 SOL 1076-43-3 C6D6

RX(7) OF 12 ...D + 3 H ==> I



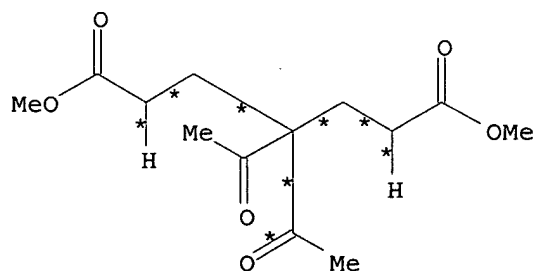
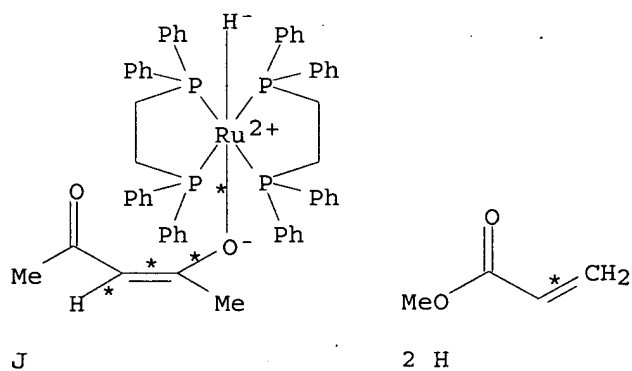
(7) \rightarrow



I
YIELD 89%

RX(7) RCT D 211634-64-9, H 96-33-3
PRO I 19766-36-0
SOL 1076-43-3 C6D6

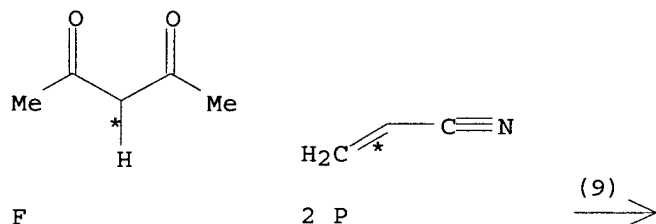
RX(8) OF 12 J + 2 H ==> K



K
YIELD 91%

RX(8) RCT J 211634-66-1, H 96-33-3
 PRO K 13984-59-3
 SOL 1076-43-3 C6D6

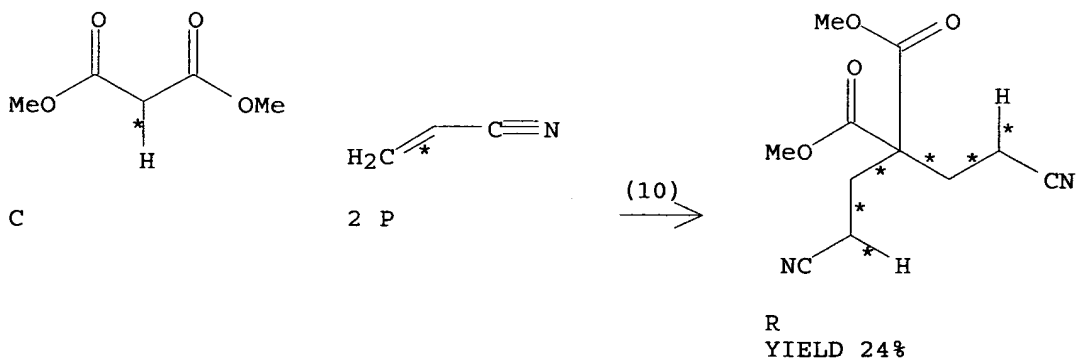
RX(9) OF 12 F + 2 P ==> Q



Q
 YIELD 70%

RX(9) RCT F 123-54-6, P 107-13-1
 PRO Q 5324-43-6
 CAT 211634-64-9 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[methyl 3-(hydroxy-κO)-3-methoxy-2-propenoato]-, (OC-6-11)-
 SOL 71-43-2 Benzene
 NTE chemoselective, yield based on 1,3-pentanedione

RX(10) OF 12 C + 2 P ==> R

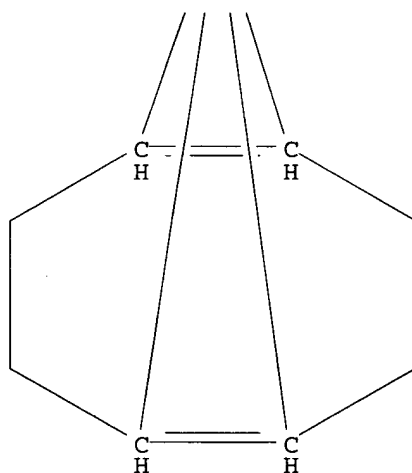


RX(10) RCT C 108-59-8, P 107-13-1
 PRO R 22711-92-8
 CAT 211634-64-9 Ruthenium, bis[1,2-ethanediylbis[diphenylphosphine-κP]]hydro[methyl 3-(hydroxy-κO)-3-methoxy-2-propenoato]-, (OC-6-11)-
 SOL 71-43-2 Benzene
 NTE chemoselective, yield based on di-Me malonate

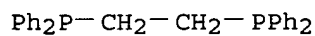
RX(12) OF 12 COMPOSED OF RX(1), RX(7)
 RX(12) A + 2 B + C + 3 H ==>
 I

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
 *

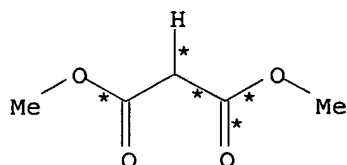
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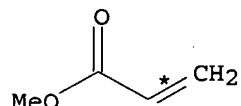
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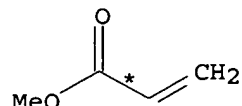
2 B



C

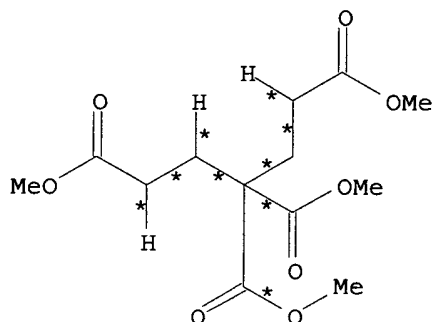


2 H



H

2
STEPS
→



I
YIELD 89%

RX(1) RCT A 42516-72-3, B 1663-45-2, C 108-59-8
PRO D 211634-64-9
SOL 71-43-2 Benzene

RX(7) RCT D 211634-64-9, H 96-33-3
PRO I 19766-36-0
SOL 1076-43-3 C6D6

L20 ANSWER 4 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 118:255103 CASREACT

TITLE: Synthesis of 2-transition-metal-substituted
1,3-butadienyl complexes with unusual
structures and facile Diels-Alder reactions of
cobalt 1,3-butadiene complexes

AUTHOR(S): Smalley, Terrence L., Jr.; Wright, Marcus W.;
Garmon, Stuart A.; Welker, Mark E.; Rheingold,
Arnold L.

CORPORATE SOURCE: Dep. Chem., Wake Forest Univ., Winston-Salem,
NC, 27109, USA

SOURCE: Organometallics (1993), 12(4), 998-1000
CODEN: ORGND7; ISSN: 0276-7333

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 29-13 (Organometallic and Organometalloidal
Compounds)

Section cross-reference(s): 24

ABSTRACT:

The cyclopentadienyliron dicarbonyl anion and (Rpy)(DMG)2Co anions (DMG = dimethylglyoximate; R = H, t-Bu) react cleanly with 1,2-butadienyl chlorides and tosylates to generate transition-metal-substituted 1,3-butadienes CH2:C(MLn)CH:CH2 [MLn = CpFe(CO)2, (py)(DMG)2Co, (4-t-Bupy)(DMG)2Co]. The cobalt-substituted 1,3-butadienes react under mild conditions and with high regioselectivity with a variety of dienophiles to yield transition-metal-substituted cyclohexenes. A

variety of cyclohexanoid products can subsequently be obtained from these transition-metal-substituted cyclohexenes via demetalation reactions.

SUPPL. TERM: Diels Alder cobalt butadiene complex; transition metal substituted butadienyl complex; cyclohexene deriv organometallic prepn

INDEX TERM: Regiochemistry
(of Diels-Alder reaction of cobalt butadiene complexes)

INDEX TERM: Diels-Alder reaction
Kinetics of Diels-Alder reaction
(of cobalt butadiene complexes)

INDEX TERM: 80-62-6, Methyl methacrylate 96-33-3, Methyl acrylate 97-63-2, Ethyl methacrylate 106-51-4, 2,5-Cyclohexadiene-1,4-dione, reactions 108-31-6, Maleic anhydride, reactions 140-88-5, Ethyl acrylate 624-48-6, Dimethyl maleate 624-49-7, Dimethyl fumarate 762-21-0, Diethyl acetylene dicarboxylate 3377-20-6 3377-21-7, Dimethyl methylene malonate

ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Diels-Alder reaction of, with cobalt-substituted butadiene)

INDEX TERM: 142617-67-2P 147735-85-1P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and Diels-Alder reactions of)

INDEX TERM: 147735-88-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and demetalation of)

INDEX TERM: 25790-55-0P 147396-58-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with transition metal anions)

INDEX TERM: 38511-09-0P 55704-60-4P 60372-92-1P
142617-59-2P 142617-60-5P 142808-86-4P
147396-57-4P 147583-82-2P 147583-83-3P
147583-84-4P 147735-86-2P 147735-87-3P
147735-89-5P 147735-90-8P 147735-91-9P
147762-44-5P 147782-96-5P 147782-97-6P
147782-98-7P
ROLE: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

INDEX TERM: 12152-20-4 75699-52-4 130351-49-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with butadienyl chloride or tosylate)

INDEX TERM: 110-86-1, Pyridine, reactions 3978-81-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cobalt chloride hexahydrate and dimethylglyoxime)

INDEX TERM: 95-45-4, Dimethylglyoxime
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with cobalt chloride hexahydrate and pyridines)

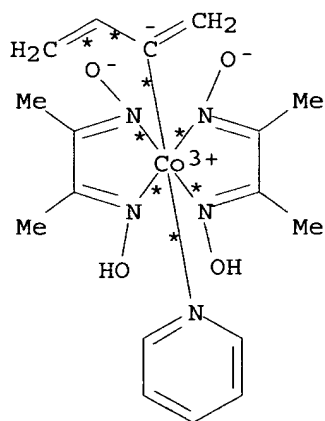
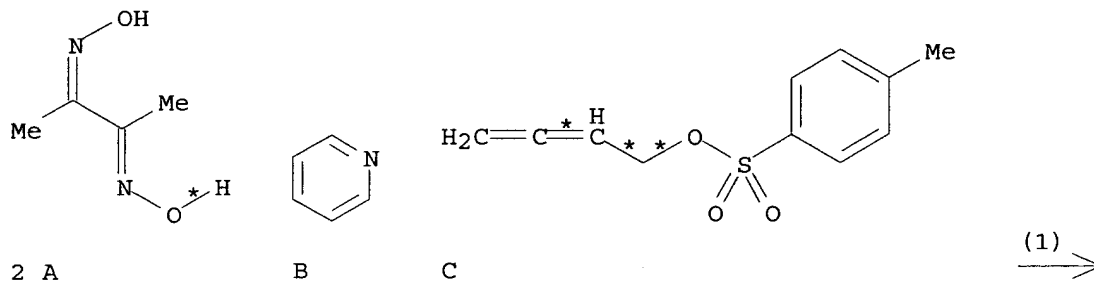
INDEX TERM: 7791-13-1 13815-10-6

ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with dimethylglyoxime and
pyridines)

INDEX TERM: 18913-31-0, 2,3-Butadien-1-ol

ROLE: RCT (Reactant); RACT (Reactant or reagent)
(reactions of)

RX(1) OF 23 2 A + B + C ==> D...



D
YIELD 75%

RX(1) RCT A 95-45-4

STAGE(1)

RGT E 13815-10-6 Cobalt(2+), hexaaqua-, dichloride,
(OC-6-11) -
SOL 67-56-1 MeOH

STAGE(2)

RCT B 110-86-1
RGT F 75-09-2 CH₂Cl₂
SOL 7732-18-5 Water

STAGE(3)

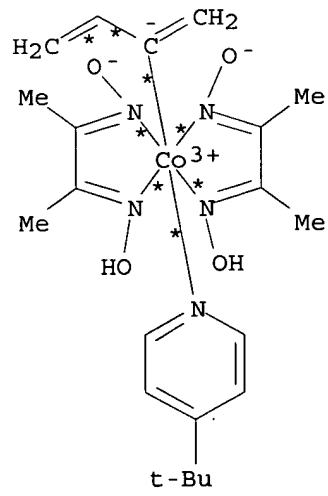
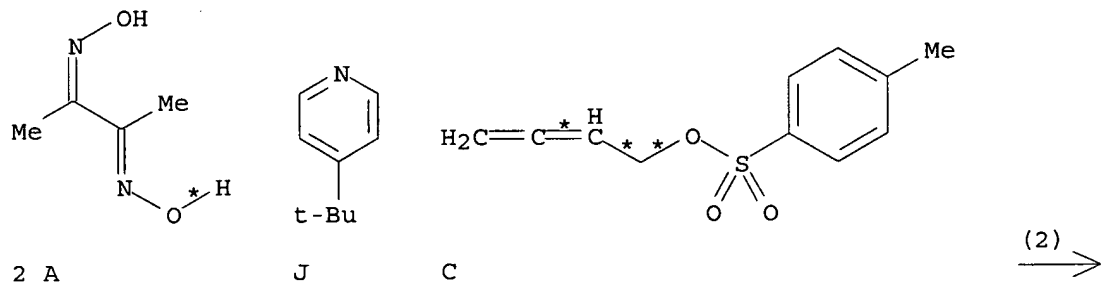
RGT G 16940-66-2 NaBH₄

SOL 7732-18-5 Water

STAGE(4)
RCT C 147396-58-5

PRO D 142617-67-2

RX(2) OF 23 2 A + J + C ==> K...



K
YIELD 58%

RX(2) RCT A 95-45-4

STAGE(1)
RGT E 13815-10-6 Cobalt(2+), hexaaqua-, dichloride,
(OC-6-11) -
SOL 67-56-1 MeOH

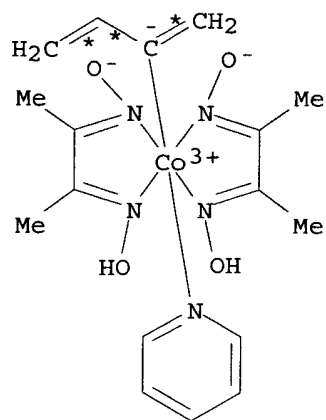
STAGE(2)
RCT J 3978-81-2
RGT F 75-09-2 CH2Cl2
SOL 7732-18-5 Water

STAGE(3)

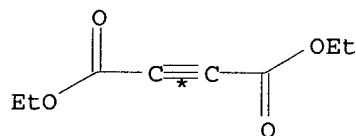
RCT C 147396-58-5
RGT G 16940-66-2 NaBH4
SOL 7732-18-5 Water

PRO K 147735-85-1

RX(3) OF 23 ...D + L ==> M



D



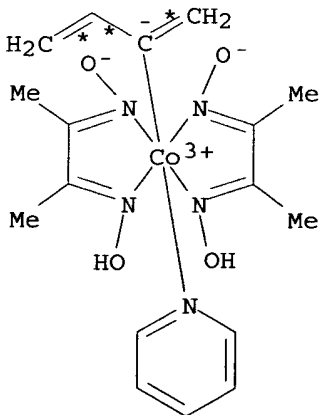
L

(3) →

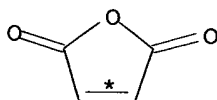
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

RX(3) RCT D 142617-67-2, L 762-21-0
PRO M 147735-86-2
SOL 109-99-9 THF

RX(4) OF 23 ...D + O ==> P

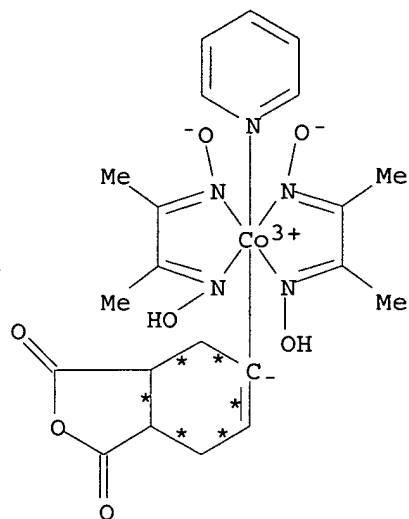


D



O

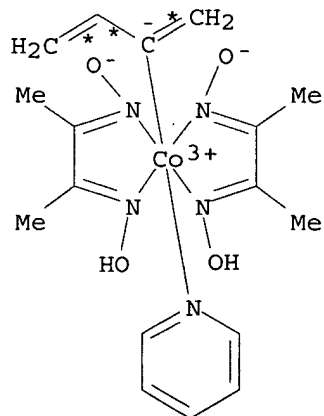
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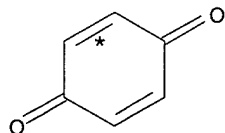
P
YIELD 80%

RX(4) RCT D 142617-67-2, O 108-31-6
PRO P 147782-96-5
SOL 109-99-9 THF

RX(5) OF 23 ...D + Q ==> R

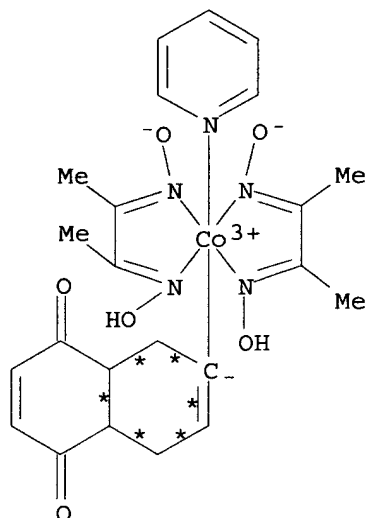


D



Q

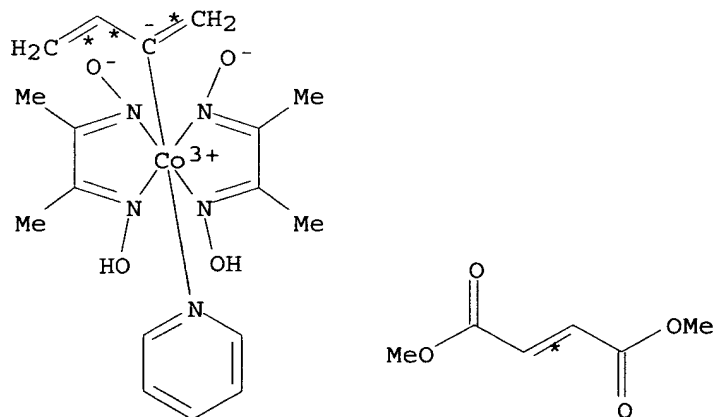
(5) →



R
YIELD 99%

RX(5) RCT D 142617-67-2, Q 106-51-4
PRO R 147782-97-6
SOL 109-99-9 THF

RX(6) OF 23 ...D + S ==> T



D

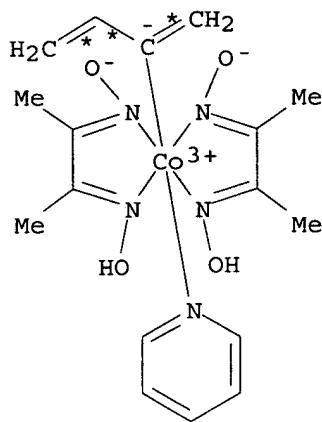
S

(6) →

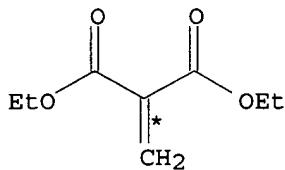
* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

RX(6) RCT D 142617-67-2, S 624-49-7
PRO T 142808-86-4
SOL 109-99-9 THF

RX(7) OF 23 ...D + U ==> V...



D



U

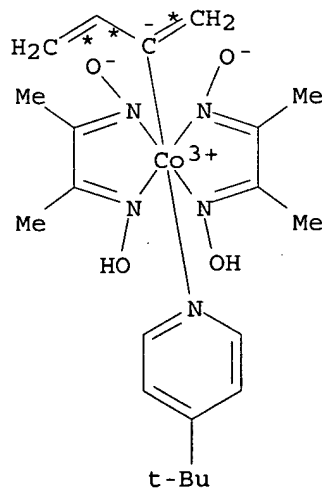
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

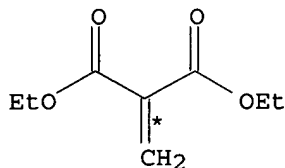
*

RX(7) RCT D 142617-67-2, U 3377-20-6
 PRO V 147735-88-4
 SOL 109-99-9 THF

RX(8) OF 23 ...K + U ==> W



K



U

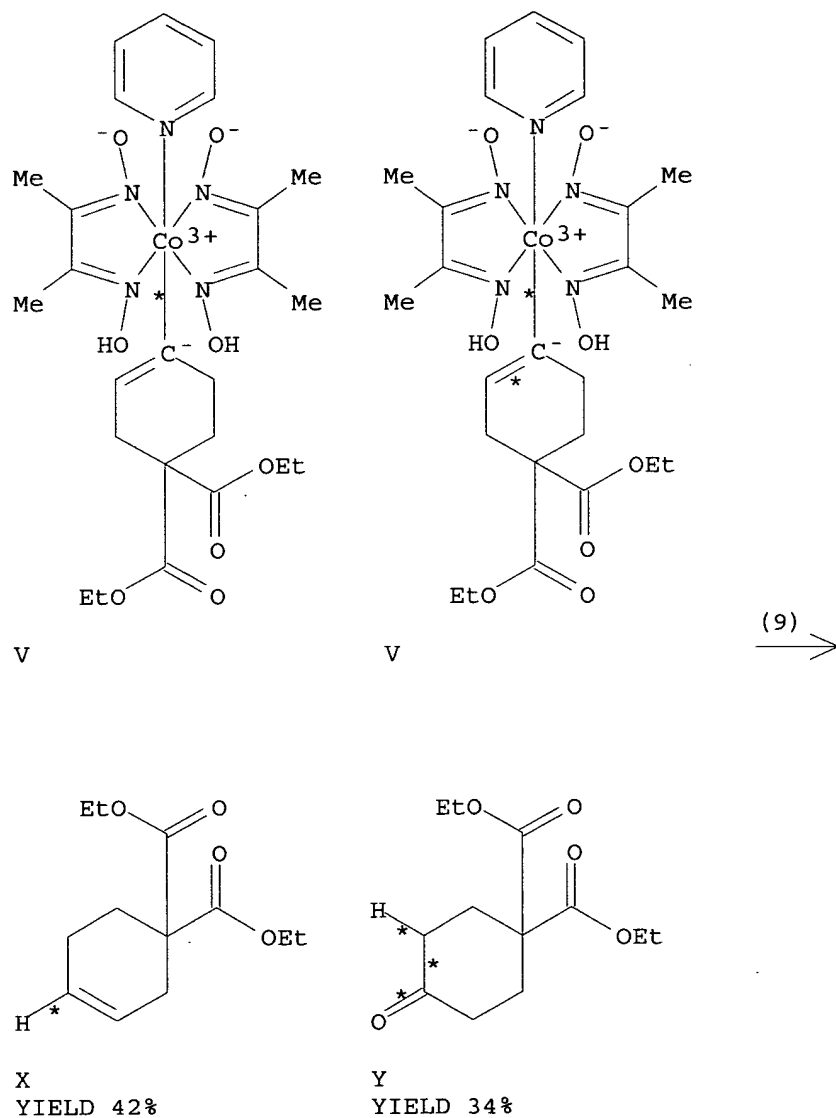
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* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

*

RX(8) RCT K 147735-85-1, U 3377-20-6
 PRO W 147735-89-5
 SOL 109-99-9 THF

RX(9) OF 23 ...2 V ==> X + Y

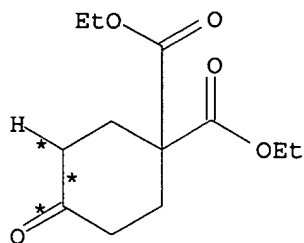


RX(9) RCT V 147735-88-4
 RGT Z 7647-01-0 HCl
 PRO X 38511-09-0, Y 55704-60-4
 SOL 75-09-2 CH₂Cl₂, 7732-18-5 Water

RX(10) OF 23 ...V ==> Y

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
*

(10)
→



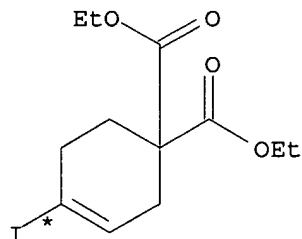
Y
YIELD 48%

RX(10) RCT V 147735-88-4
RGT Z 7647-01-0 HCl, AA 7722-84-1 H2O2
PRO Y 55704-60-4
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

RX(11) OF 23 ...V ==> AB

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT
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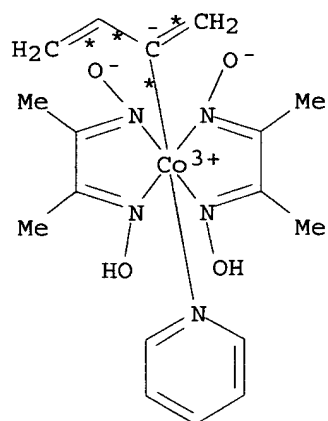
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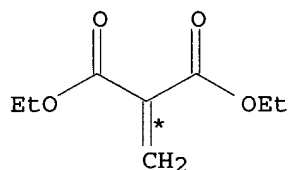
AB
YIELD 76%

RX(11) RCT V 147735-88-4
RGT AC 7553-56-2 I2
PRO AB 147396-57-4
SOL 75-09-2 CH2Cl2

RX(18) OF 23 COMPOSED OF RX(7), RX(9)
RX(18) 2 D + 2 U ==> X + Y

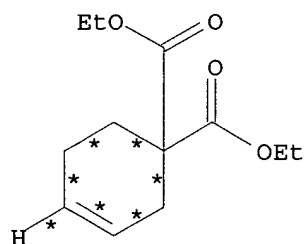


2 D

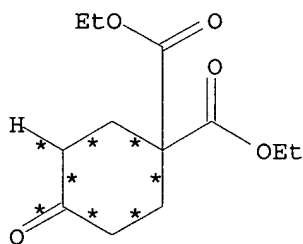


2 U

2
STEPS
→



X
YIELD 42%



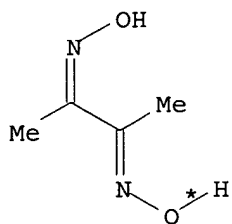
Y
YIELD 34%

RX (7) RCT D 142617-67-2, U 3377-20-6
PRO V 147735-88-4
SOL 109-99-9 THF

RX (9) RCT V 147735-88-4
RGT Z 7647-01-0 HCl
PRO X 38511-09-0, Y 55704-60-4
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

RX (21) OF 23 COMPOSED OF RX (1), RX (7), RX (9)

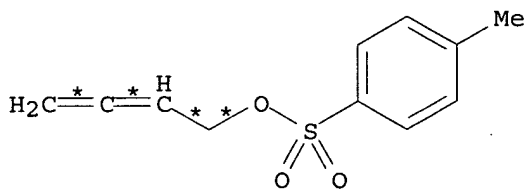
RX (21) 4 A + 2 B + 2 C + 2 U ==> X + Y



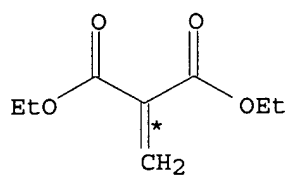
4 A



2 B

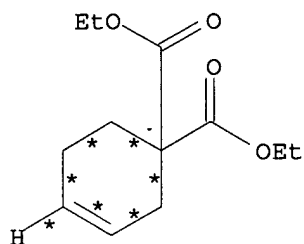


2 C

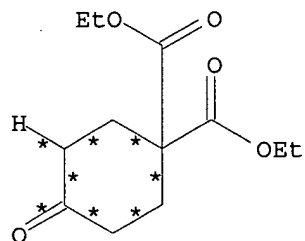


2 U

3
STEPS
→



X
YIELD 42%



Y
YIELD 34%

RX(1) RCT A 95-45-4

STAGE(1)

RGT E 13815-10-6 Cobalt(2+), hexaaqua-,
dichloride, (OC-6-11)-
SOL 67-56-1 MeOH

STAGE(2)

RCT B 110-86-1
RGT F 75-09-2 CH2Cl2
SOL 7732-18-5 Water

STAGE(3)

RGT G 16940-66-2 NaBH4
SOL 7732-18-5 Water

STAGE(4)

RCT C 147396-58-5

PRO D 142617-67-2

RX(7) RCT D 142617-67-2, U 3377-20-6
PRO V 147735-88-4
SOL 109-99-9 THF

RX(9) RCT V 147735-88-4
RGT Z 7647-01-0 HCl
PRO X 38511-09-0, Y 55704-60-4
SOL 75-09-2 CH2Cl2, 7732-18-5 Water

L20 ANSWER 5 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 111:195366 CASREACT

TITLE: Palladium(II)-assisted carboacylation of
enamides to produce functionalized
 β -amino acids. Synthesis of relays to
(\pm)-thienamycin

AUTHOR(S): Wieber, Gary M.; Hegedus, Louis S.; Akermark,
Bjorn; Michalson, Erik T.

CORPORATE SOURCE: Dep. Chem., Colorado State Univ., Fort
Collins, CO, 80523, USA

SOURCE: Journal of Organic Chemistry (1989), 54(19),
4649-53

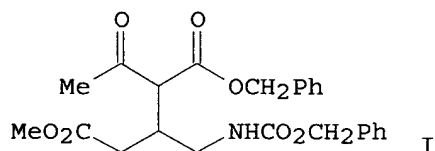
CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

CLASSIFICATION: 34-2 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 26

GRAPHIC IMAGE:



ABSTRACT:

Alkylation of benzyl vinylcarbamate with sodium benzyl acetoacetate in the presence of palladium(II) chloride, followed by carbonylation (CO/MeOH), produced a highly functionalized β -amido ester I, which was converted, using conventional organic synthetic methodol., into a relay to (\pm)-thienamycin.

SUPPL. TERM: palladium carboacylation enamide; beta amino acid
functionalized; thienamycin relay; lactam beta

INDEX TERM: Acylation
(of enamides in presence of palladium,
functionalized β -amino acids from)

INDEX TERM: Amides, reactions

ROLE: RCT (Reactant); RACT (Reactant or reagent)
(unsatd., palladium-assisted carboacylation of,

functionalized β -amino acids from)
INDEX TERM: Amino acids, preparation
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(β -, preparation of, by palladium-assisted
carboacylation of enamides)
INDEX TERM: Lactams
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(β -, preparation of, palladium-assisted
carboacylation of enamides to produce
functionalized β -amino acids in relation to)
INDEX TERM: 122313-67-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(alkylation by, of benzyl vinylcarbamate in
presence of palladium chloride)
INDEX TERM: 7440-05-3, Palladium, uses and miscellaneous
ROLE: USES (Uses)
(carboacylation of enamides in presence of,
functionalized β -amino acids from)
INDEX TERM: 84713-20-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and alkylation of, with sodium benzyl
acetoacetate in presence of palladium chloride,
carbonylation of product from)
INDEX TERM: 122313-57-9P 122313-59-1P 122313-60-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and cyclocondensation of, β -lactam
from)
INDEX TERM: 122313-64-8P 122313-65-9P
ROLE: SPN (Synthetic preparation); PREP
(Preparation)
(preparation and deketalization)
INDEX TERM: 122313-61-5P 122313-62-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and deketalization or silylation of)
INDEX TERM: 122313-55-7P 122313-56-8P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydride reduction of)
INDEX TERM: 122313-69-3P 122313-70-6P 122313-71-7P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and hydrogenolysis of)
INDEX TERM: 50830-56-3P, Acryloyl azide
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction of, with benzyl alc.)
INDEX TERM: 122313-63-7P 122332-75-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and reduction of)
INDEX TERM: 86421-11-6P 106248-39-9P 122313-68-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and O-silylation of, with
tert-butyldimethylsilyl chloride)

INDEX TERM: 86421-12-7P 93711-82-1P 122313-53-5P
 122313-54-6P 122313-66-0P 122405-37-2P
 136353-97-4P
 ROLE: SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation of)

INDEX TERM: 65750-57-4
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (preparation of relays to, palladium-assisted
 carboacylation of enamides to produce
 functionalized β -amino acids in relation to)

INDEX TERM: 100-51-6, Benzenemethanol, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with acryloyl azide)

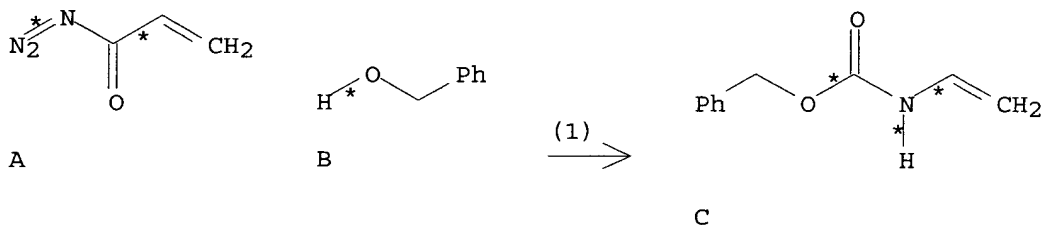
INDEX TERM: 814-68-6, 2-Propenoyl chloride
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with azide)

INDEX TERM: 609-08-5, Diethyl methylmalonate
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with benzyl vinylcarbamate
 palladium complex)

INDEX TERM: 69739-34-0, tert-Butyldimethylsilyl triflate
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (N-silylation by, of β -lactam)

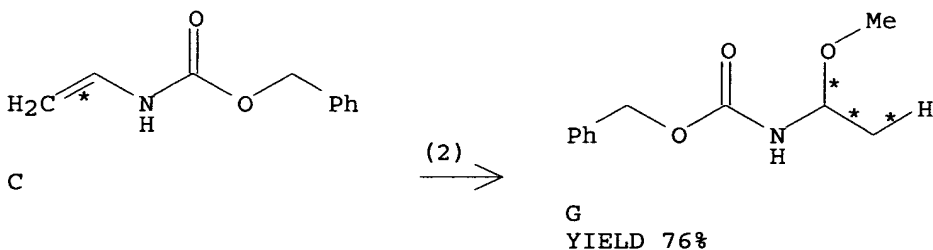
INDEX TERM: 18162-48-6, tert-Butyldimethylsilyl chloride
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (O-silylation by, of hydroxyhexanoic acid derivative)

RX(1) OF 100 ...A + B ==> C...



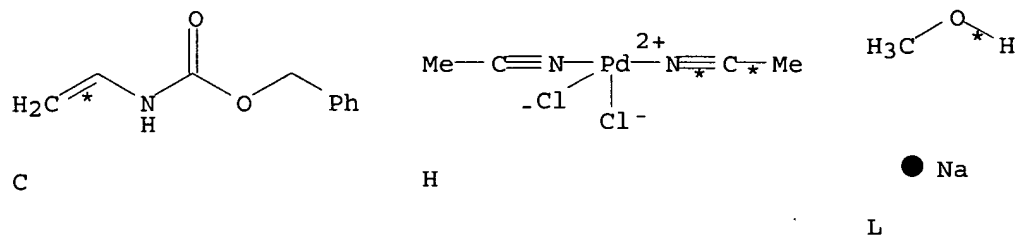
RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(2) OF 100 ...C ==> G



RX(2) RCT C 84713-20-2
 RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8 Et₃N, J 1333-74-0
 H₂, K 67-56-1 MeOH
 PRO G 136353-97-4
 SOL 67-56-1 MeOH

RX(3) OF 100 ...C + H + L ==> M



RX(3) RCT C 84713-20-2, H 14592-56-4

STAGE(1)

SOL 109-99-9 THF

STAGE(2)

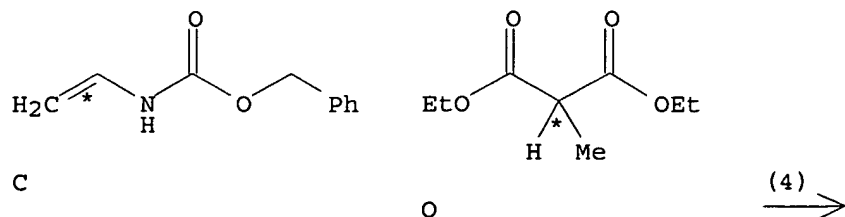
RCT L 124-41-4

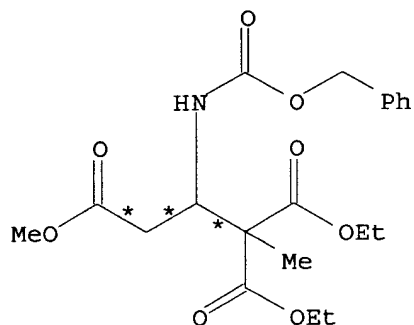
RGT I 121-44-8 Et₃N

SOL 109-99-9 THF

PRO M 122313-53-5

RX(4) OF 100 ...C + O ==> P





P
YIELD 63%

RX(4) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂

SOL 109-99-9 THF

STAGE(2)

RCT O 609-08-5

RGT Q 16940-66-2 NaBH₄

SOL 109-99-9 THF

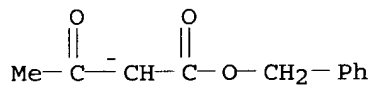
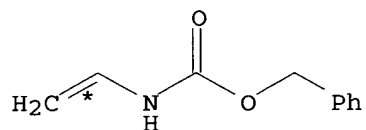
STAGE(3)

RGT I 121-44-8 Et₃N

SOL 109-99-9 THF

PRO P 122313-54-6

RX(5) OF 100 ...2 C + 2 R ==> S + T...

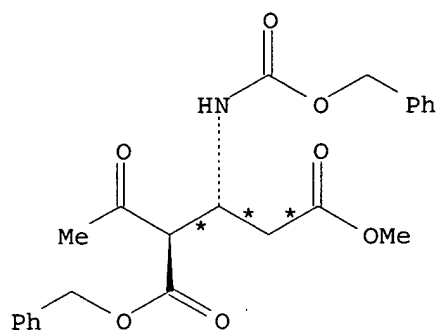


2 C

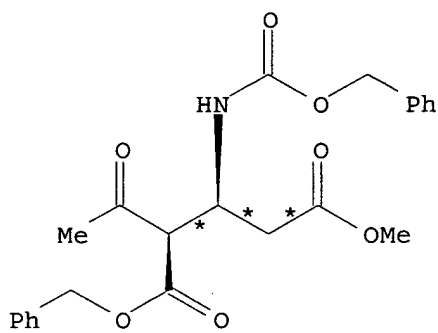
● Na⁺

2 R

(5) →



S
YIELD 92% (50)



T
YIELD 92% (50)

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8 Et₃N
SOL 109-99-9 THF

STAGE(2)

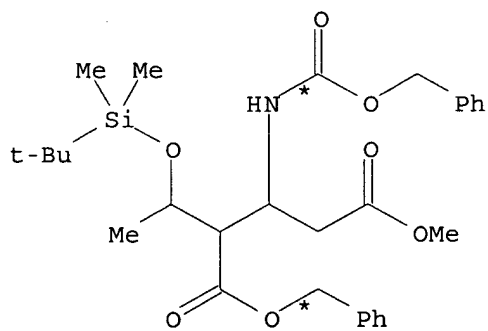
RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

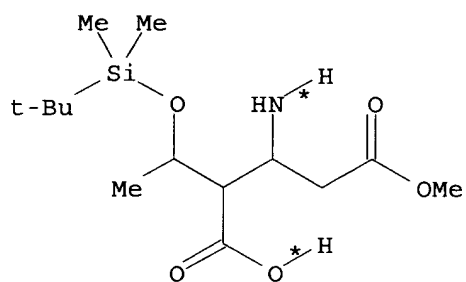
PRO S 122313-55-7, T 122313-56-8

RX(6) OF 100 ...V ==> W...



V

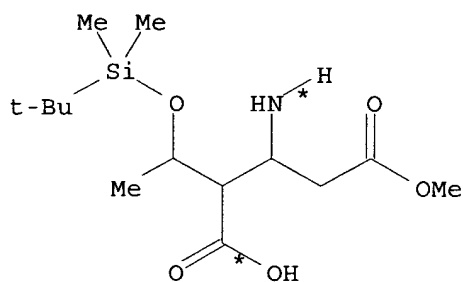
(6)
→



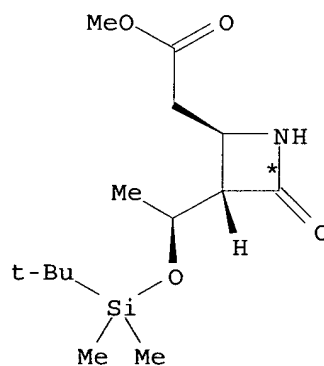
W
YIELD 95%

RX(6) RCT V 122313-69-3
 RGT J 1333-74-0 H2
 PRO W 122313-57-9
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH

RX(7) OF 100 ...W ==> Y



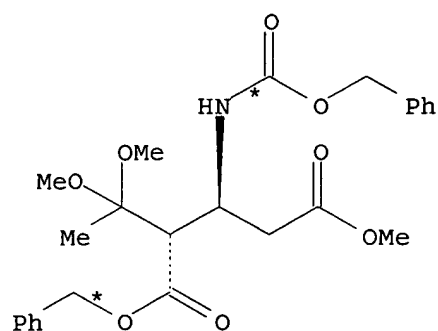
W



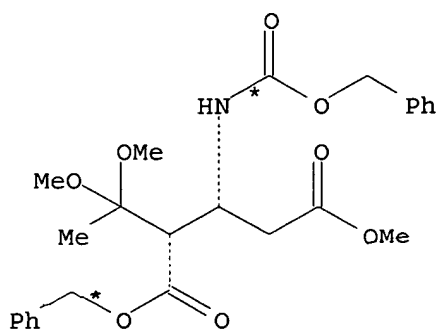
Y
YIELD 95%

RX(7) RCT W 122313-57-9
 RGT Z 538-75-0 DCC
 PRO Y 86421-12-7
 SOL 109-99-9 THF

RX(8) OF 100 ...AA + AB ==> AC + AD...

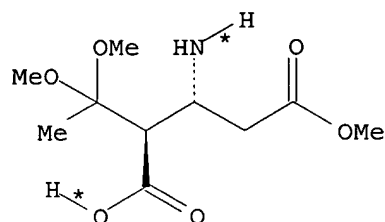


AA

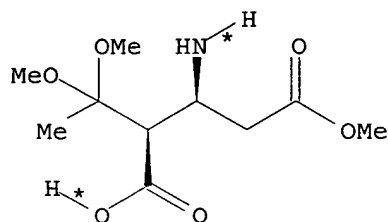


AB

(8) →



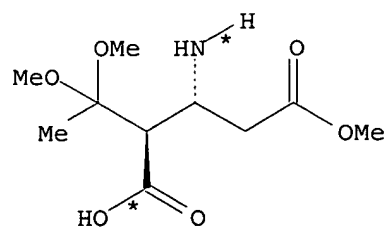
AC



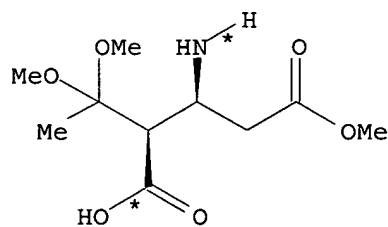
AD

RX(8) RCT AA 122313-70-6, AB 122313-71-7
 RGT J 1333-74-0 H2
 PRO AC 122313-59-1, AD 122313-60-4
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 NTE 94% overall

RX(9) OF 100 ...AC + AD ==> AE + AF...

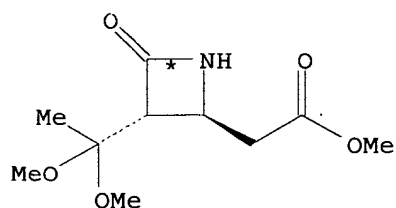


AC

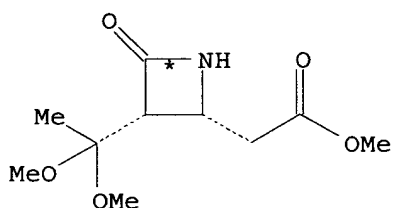


AD

(9) →



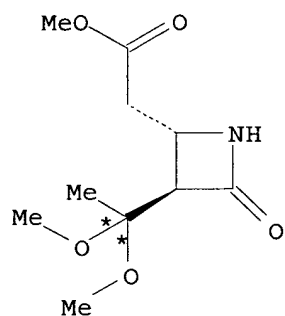
AE
YIELD 82%



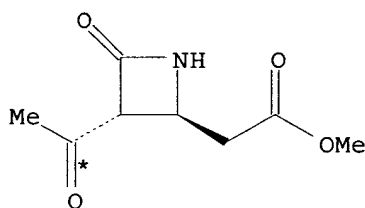
AF
YIELD 15%

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

RX(10) OF 100 ...AE ==> AG...



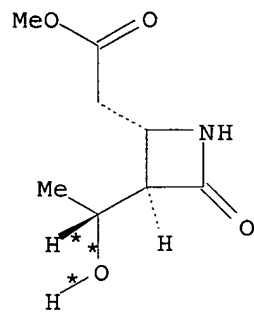
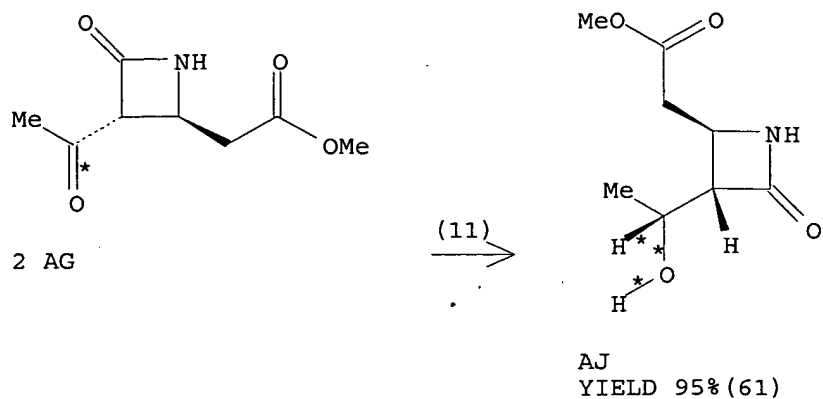
AE



AG

RX(10) RCT AE 122313-61-5
RGT AH 24057-28-1 Pyridinium tosylate
PRO AG 122313-63-7
SOL 67-64-1 Me2CO

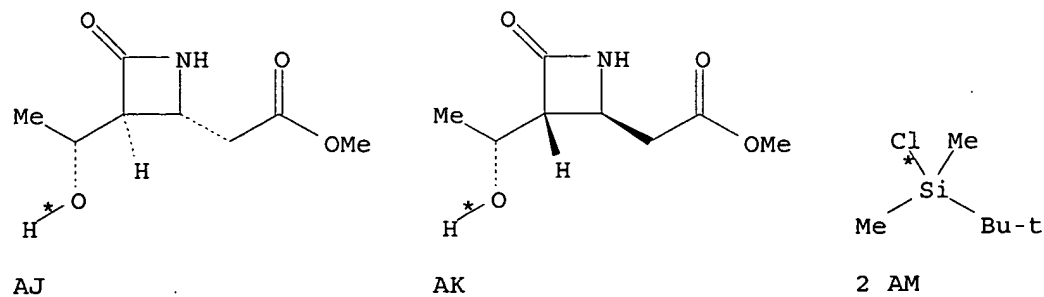
RX(11) OF 100 ...2 AG ==> AJ + AK...

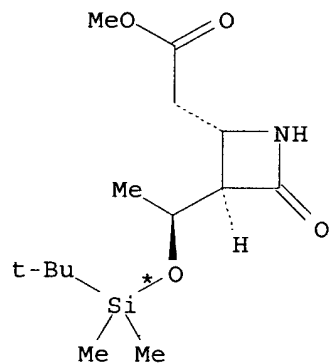
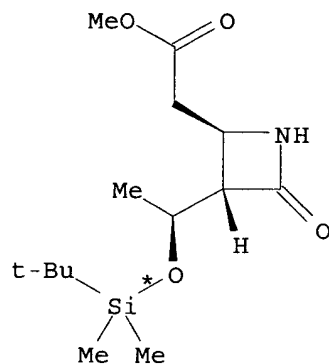


AK
YIELD 95% (39)

RX(11) RCT AG 122313-63-7
 RGT AL 54575-49-4 K Selectride
 PRO AJ 106248-39-9, AK 86421-11-6
 SOL 109-99-9 THF

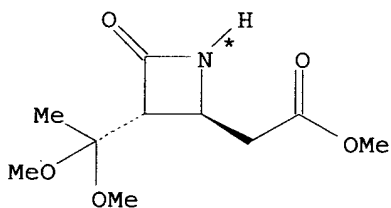
RX(12) OF 100 ...AJ + AK + 2 AM ==> AN + Y



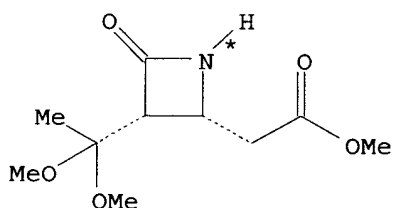
(12)
→AN
YIELD 70% (61)Y
YIELD 70% (39)

RX(12) RCT AJ 106248-39-9, AK 86421-11-6, AM 18162-48-6
 RGT AO 288-32-4 1H-Imidazole
 PRO AN 93711-82-1, Y 86421-12-7
 SOL 68-12-2 DMF

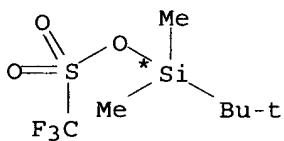
RX(13) OF 100 ...AE + AF + 2 AQ ==> AR + AS...



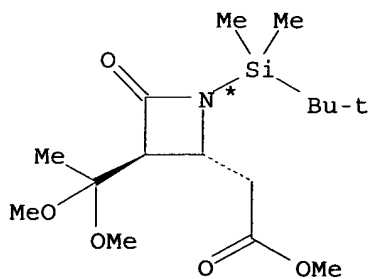
AE



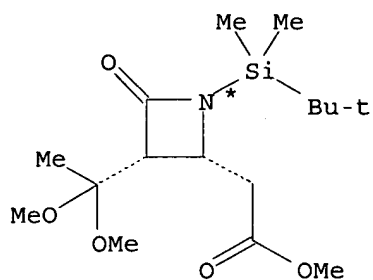
AF



2 AQ

(13)
→

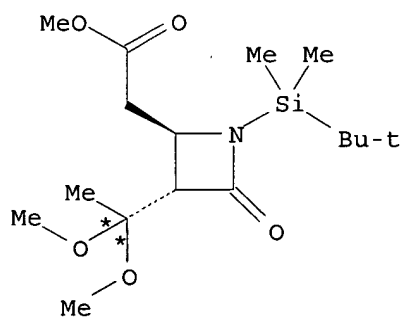
AR



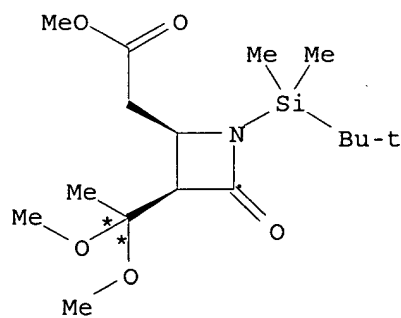
AS

RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
 RGT AT 108-48-5 2,6-Lutidine
 PRO AR 122313-64-8, AS 122313-65-9
 SOL 75-09-2 CH₂Cl₂

RX(14) OF 100 ...AR + AS ==> 2 AV...

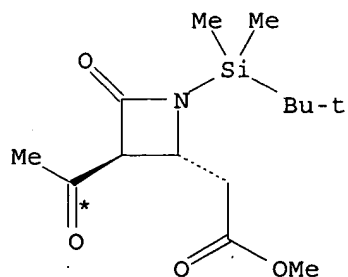


AR

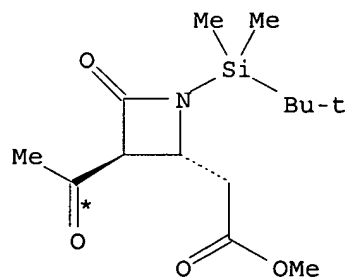


AS

(14) →



AV
YIELD 100%

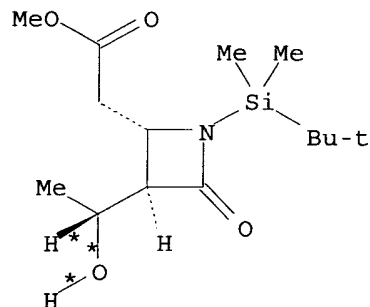
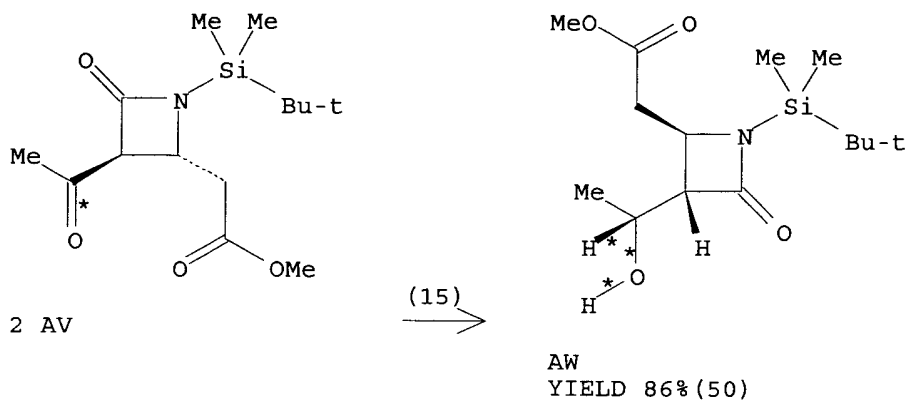


AV
YIELD 100%

RX(14) RCT AR 122313-64-8, AS 122313-65-9

RGT AH 24057-28-1 Pyridinium tosylate
 PRO AV 122332-75-6
 SOL 67-64-1 Me₂CO

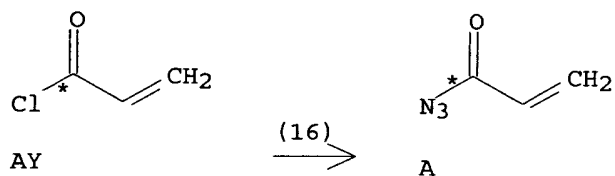
RX(15) OF 100 ...2 AV ==> AW + AX



AX
YIELD 86% (50)

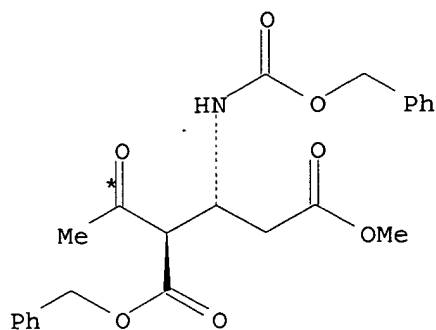
RX(15) RCT AV 122332-75-6
 RGT AL 54575-49-4 K Selectride
 PRO AW 122313-66-0, AX 122405-37-2
 SOL 109-99-9 THF

RX(16) OF 100 AY ==> A...

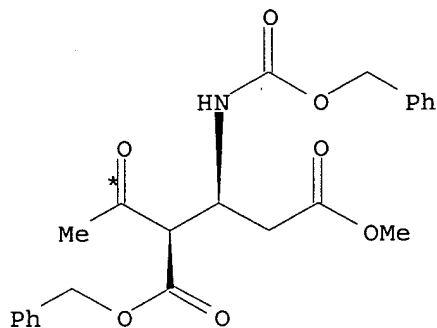


RX(16) RCT AY 814-68-6
 RGT AZ 26628-22-8 NaN₃
 PRO A 50830-56-3
 SOL 108-88-3 PhMe, 7732-18-5 Water

RX(17) OF 100 ...S + T ==> 2 BB...

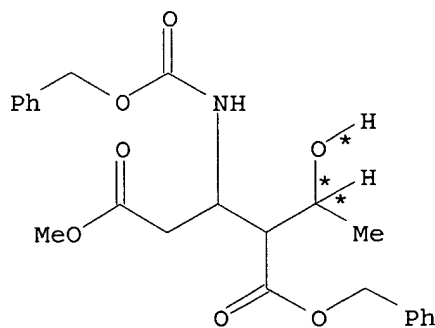


S

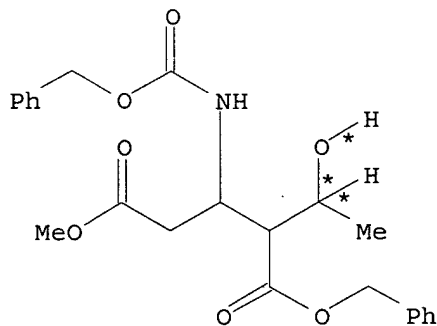


T

(17) →



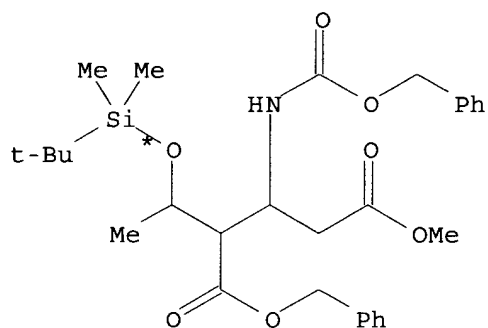
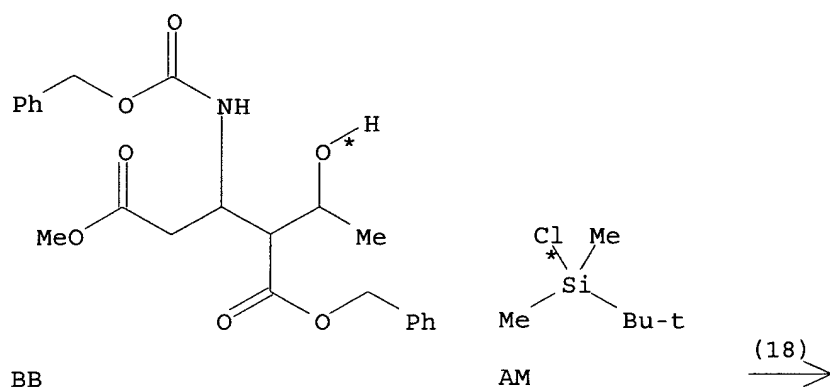
BB
 YIELD 92%



BB
 YIELD 92%

RX(17) RCT S 122313-55-7, T 122313-56-8
 RGT Q 16940-66-2 NaBH₄
 PRO BB 122313-68-2
 SOL 67-56-1 MeOH

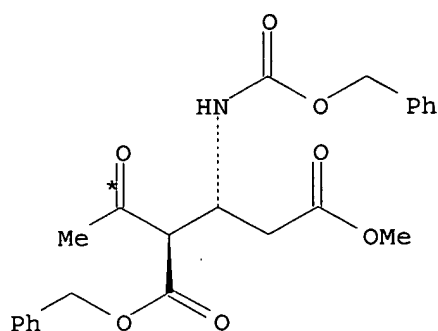
RX(18) OF 100 ...BB + AM ==> V...



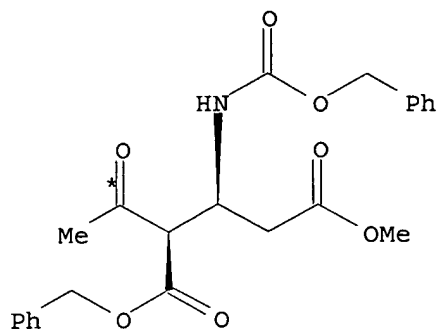
YIELD 77%

RX(18) RCT BB 122313-68-2, AM 18162-48-6
 RGT AO 288-32-4 1H-Imidazole
 PRO V 122313-69-3
 SOL 68-12-2 DMF

RX(19) OF 100 ...S + T ==> AA + AB...

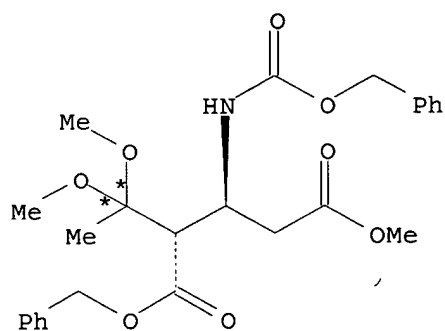


S

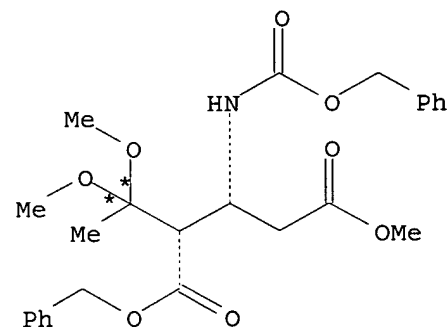


T

(19) →



AA

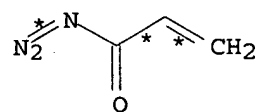


AB

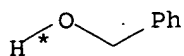
RX(19) RCT S 122313-55-7, T 122313-56-8
 RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
 PRO AA 122313-70-6, AB 122313-71-7
 SOL 67-56-1 MeOH
 NTE 90% overall

RX(22) OF 100 COMPOSED OF RX(1), RX(4)

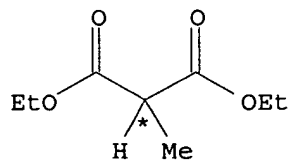
RX(22) A + B + O ==> P



A

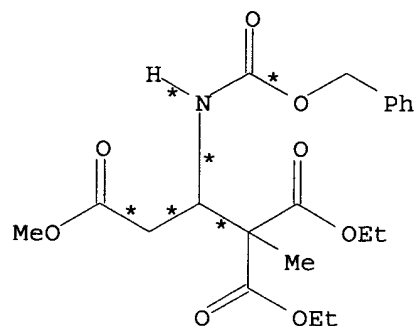


B



O

2
STEPS
→



P
YIELD 63%

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(4) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂
SOL 109-99-9 THF

STAGE(2)

RCT O 609-08-5
RGT Q 16940-66-2 NaBH₄
SOL 109-99-9 THF

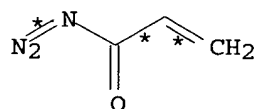
STAGE(3)

RGT I 121-44-8 Et₃N
SOL 109-99-9 THF

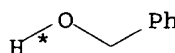
PRO P 122313-54-6

RX(23) OF 100 COMPOSED OF RX(1), RX(5)

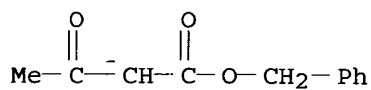
RX(23) 2 A + 2 B + 2 R ==> S +
T



2 A



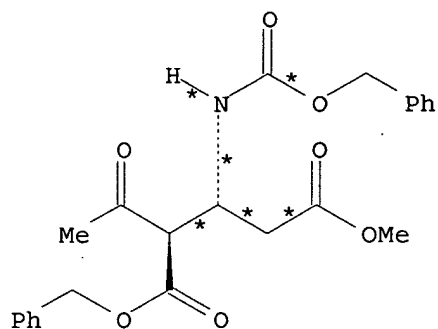
2 B



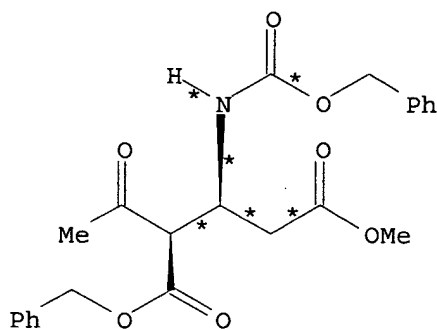
2 R

● Na⁺

2
STEPS
→



S
YIELD 92% (50)



T
YIELD 92% (50)

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
Et₃N
SOL 109-99-9 THF

STAGE(2)

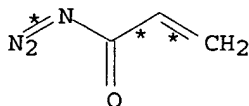
RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

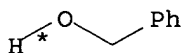
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

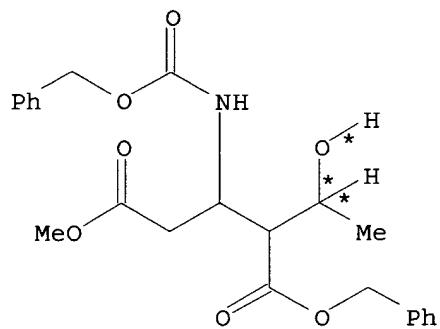
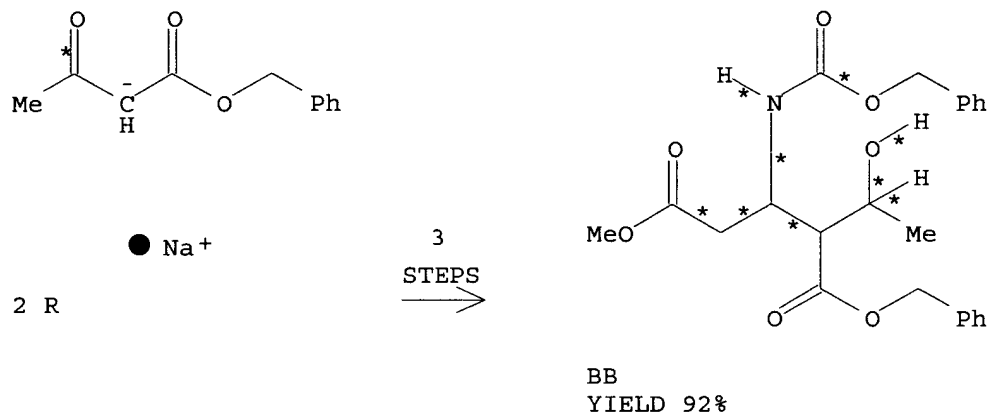
RX(38) OF 100 COMPOSED OF RX(1), RX(5), RX(17)
RX(38) 2 A + 2 B + 2 R ==> 2 BB



2 A



2 B



BB
YIELD 92%

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
 Et₃N
 SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
 SOL 109-99-9 THF

STAGE(3)

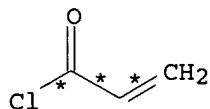
RGT K 67-56-1 MeOH, U 630-08-0 CO
 SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

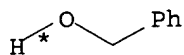
RX(17) RCT S 122313-55-7, T 122313-56-8
 RGT Q 16940-66-2 NaBH₄
 PRO BB 122313-68-2
 SOL 67-56-1 MeOH

RX(40) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(17)

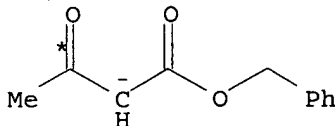
RX(40) 2 AY + 2 B + 2 R ==> 2 BB



2 AY



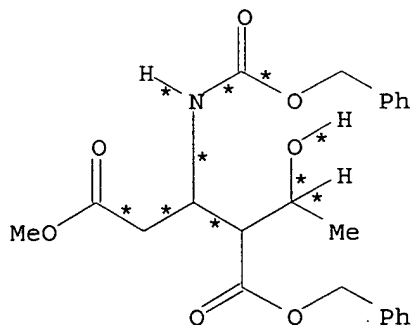
2 B



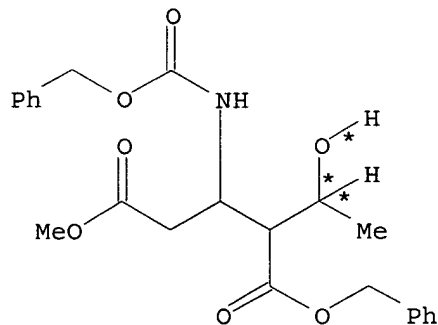
● Na⁺

2 R

4
 STEPS



BB
 YIELD 92%



BB
 YIELD 92%

RX(16) RCT AY 814-68-6
 RGT AZ 26628-22-8 NaN₃
 PRO A 50830-56-3
 SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
 Et₃N

SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
SOL 109-99-9 THF

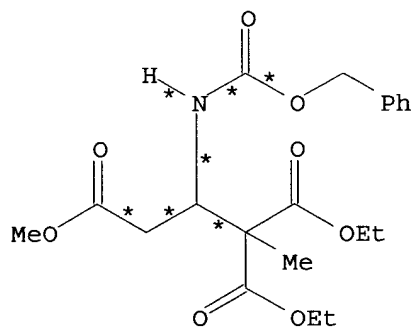
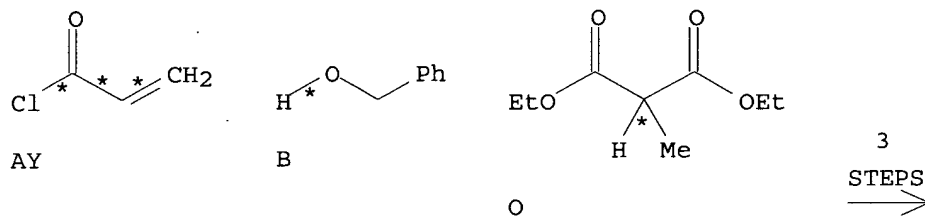
STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(17) RCT S 122313-55-7, T 122313-56-8
RGT Q 16940-66-2 NaBH4
PRO BB 122313-68-2
SOL 67-56-1 MeOH

RX(60) OF 100 COMPOSED OF RX(16), RX(1), RX(4)
RX(60) AY + B + O ==> P



P
YIELD 63%

RX(16) RCT AY 814-68-6
RGT AZ 26628-22-8 NaN3
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(4) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂
 SOL 109-99-9 THF

STAGE(2)

RCT O 609-08-5
 RGT Q 16940-66-2 NaBH₄
 SOL 109-99-9 THF

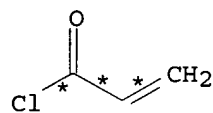
STAGE(3)

RGT I 121-44-8 Et₃N
 SOL 109-99-9 THF

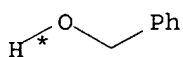
PRO P 122313-54-6

RX(61) OF 100 COMPOSED OF RX(16), RX(1), RX(5)

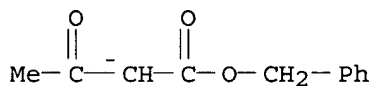
RX(61) 2 AY + 2 B + 2 R ==> S
 + T



2 AY



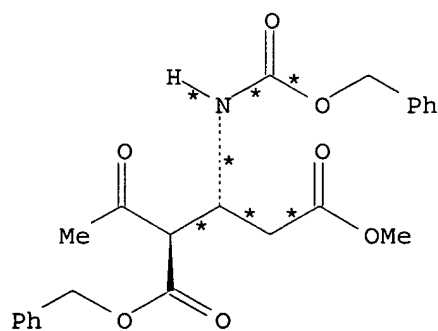
2 B



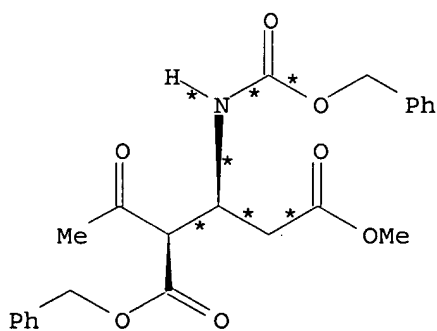
2 R



3
 STEPS
 →



S
 YIELD 92% (50)



T
 YIELD 92% (50)

RX(16) RCT AY 814-68-6
 RGT AZ 26628-22-8 NaN₃
 PRO A 50830-56-3
 SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine

PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
Et₃N
SOL 109-99-9 THF

STAGE(2)

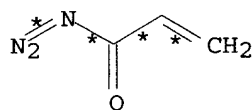
RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

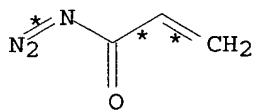
RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

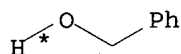
RX(77) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(10)
RX(77) 2 A + 2 B + 2 R ==> AG



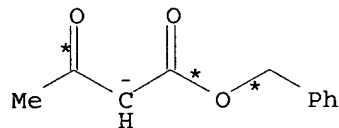
A



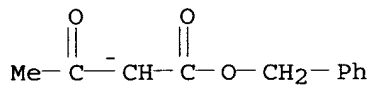
A



2 B



R

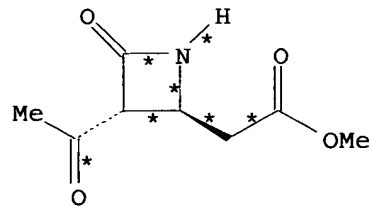


R

● Na⁺

● Na⁺

6
STEPS
→



AG

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
 Et₃N
 SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
 SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
 SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
 RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
 PRO AA 122313-70-6, AB 122313-71-7
 SOL 67-56-1 MeOH
 NTE 90% overall

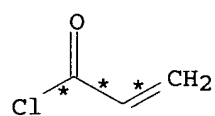
RX(8) RCT AA 122313-70-6, AB 122313-71-7
 RGT J 1333-74-0 H₂
 PRO AC 122313-59-1, AD 122313-60-4
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
 RGT Z 538-75-0 DCC
 PRO AE 122313-61-5, AF 122313-62-6
 SOL 109-99-9 THF

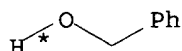
RX(10) RCT AE 122313-61-5
 RGT AH 24057-28-1 Pyridinium tosylate
 PRO AG 122313-63-7
 SOL 67-64-1 Me₂CO

RX(80) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
 RX(10)

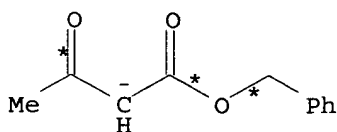
RX(80) 2 AY + 2 B + 2 R ==> AG



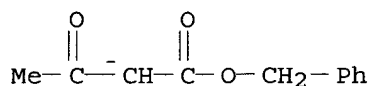
2 AY



2 B

● Na⁺

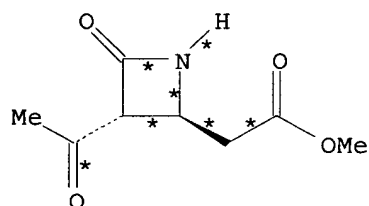
R

● Na⁺

7

STEPS

R



AG

RX(16) RCT AY 814-68-6
 RGT AZ 26628-22-8 NaN₃
 PRO A 50830-56-3
 SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
 RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
 Et₃N
 SOL 109-99-9 THF

STAGE(2)
 RCT R 122313-67-1
 SOL 109-99-9 THF

STAGE(3)
 RGT K 67-56-1 MeOH, U 630-08-0 CO
 SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
 RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
 PRO AA 122313-70-6, AB 122313-71-7
 SOL 67-56-1 MeOH
 NTE 90% overall

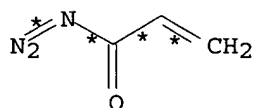
RX(8) RCT AA 122313-70-6, AB 122313-71-7
 RGT J 1333-74-0 H2
 PRO AC 122313-59-1, AD 122313-60-4
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
 RGT Z 538-75-0 DCC
 PRO AE 122313-61-5, AF 122313-62-6
 SOL 109-99-9 THF

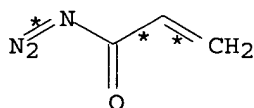
RX(10) RCT AE 122313-61-5
 RGT AH 24057-28-1 Pyridinium tosylate
 PRO AG 122313-63-7
 SOL 67-64-1 Me2CO

RX(93) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(10),
 RX(11)

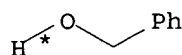
RX(93) 3 A + B + 3 R ==> AJ +
 AK



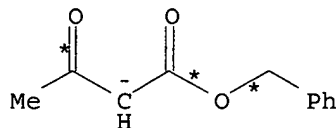
2 A



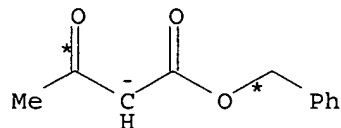
A



B

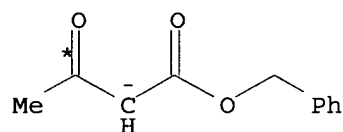


R



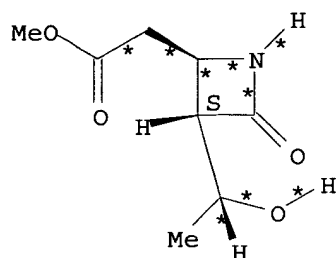
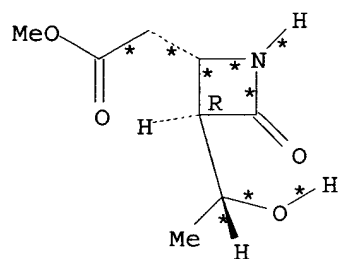
R

● Na⁺● Na⁺

● Na⁺

7

STEPS

AJ
YIELD 95% (61)AK
YIELD 95% (39)

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
 Et₃N
 SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
 SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
 SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
 RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
 PRO AA 122313-70-6, AB 122313-71-7
 SOL 67-56-1 MeOH
 NTE 90% overall

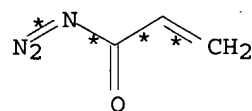
RX(8) RCT AA 122313-70-6, AB 122313-71-7
 RGT J 1333-74-0 H2
 PRO AC 122313-59-1, AD 122313-60-4
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
 RGT Z 538-75-0 DCC
 PRO AE 122313-61-5, AF 122313-62-6
 SOL 109-99-9 THF

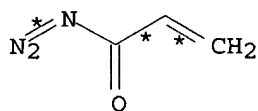
RX(10) RCT AE 122313-61-5
 RGT AH 24057-28-1 Pyridinium tosylate
 PRO AG 122313-63-7
 SOL 67-64-1 Me2CO

RX(11) RCT AG 122313-63-7
 RGT AL 54575-49-4 K Selectride
 PRO AJ 106248-39-9, AK 86421-11-6
 SOL 109-99-9 THF

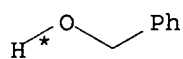
RX(94) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(13),
 RX(14)
 RX(94) 2 A + B + 2 R + 2 AQ ==> 2
 AV



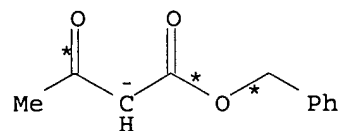
A



A

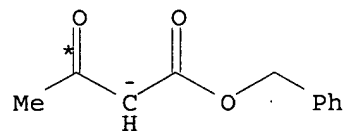


B



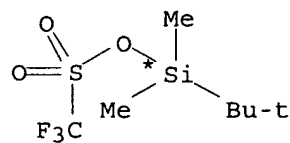
● Na⁺

R



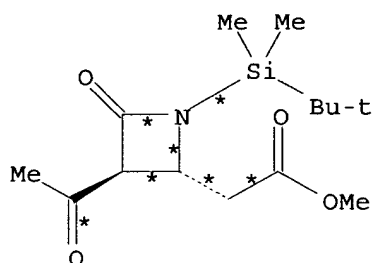
● Na⁺

R

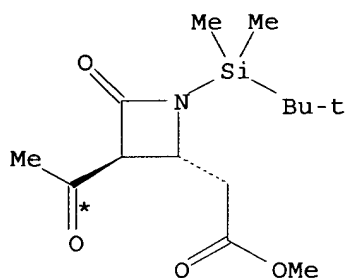


2 AQ

7
STEPS
→



AV
YIELD 100%



AV
YIELD 100%

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
Et₃N
SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H₂
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

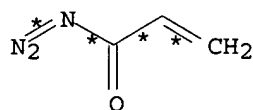
RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine
PRO AR 122313-64-8, AS 122313-65-9

SOL 75-09-2 CH2Cl2

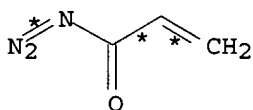
RX(14) RCT AR 122313-64-8, AS 122313-65-9
 RGT AH 24057-28-1 Pyridinium tosylate
 PRO AV 122332-75-6
 SOL 67-64-1 Me2CO

RX(96) OF 100 COMPOSED OF RX(1), RX(5), RX(19), RX(8), RX(9), RX(13),
 RX(14), RX(15)

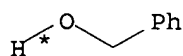
RX(96) 3 A + B + 3 R + 3 AQ ==>
 AW + AX



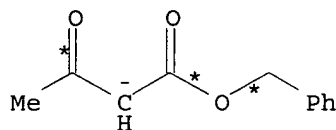
2 A



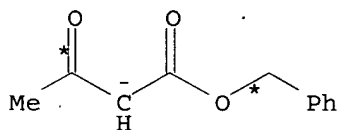
A



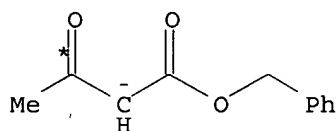
B



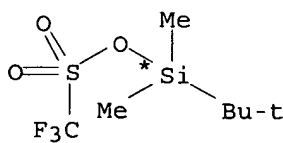
R

● Na⁺

R

● Na⁺

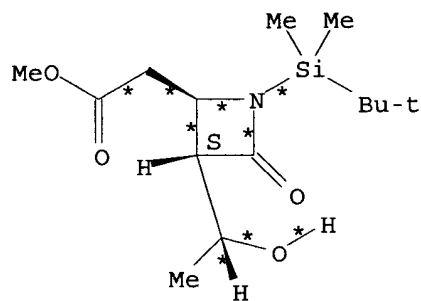
R

● Na⁺

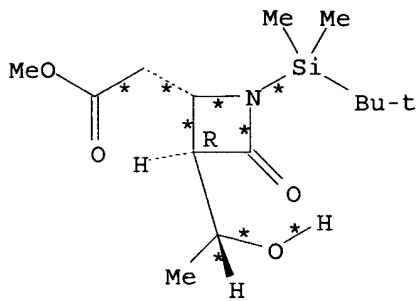
3 AQ

8

STEPS
→



AW
YIELD 86%(50)



AX
YIELD 86%(50)

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl2(MeCN)2, I 121-44-8
Et3N
SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H2
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine

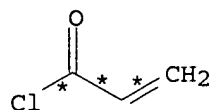
PRO AR 122313-64-8, AS 122313-65-9
SOL 75-09-2 CH₂Cl₂

RX(14) RCT AR 122313-64-8, AS 122313-65-9
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV 122332-75-6
SOL 67-64-1 Me₂CO

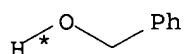
RX(15) RCT AV 122332-75-6
RGT AL 54575-49-4 K Selectride
PRO AW 122313-66-0, AX 122405-37-2
SOL 109-99-9 THF

RX(97) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
RX(10), RX(11)

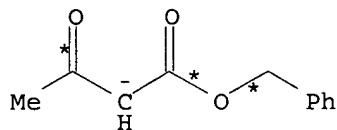
RX(97) 3 AY + 3 B + 3 R ==> AJ
+ AK



3 AY

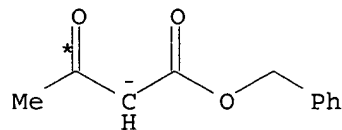


3 B



R

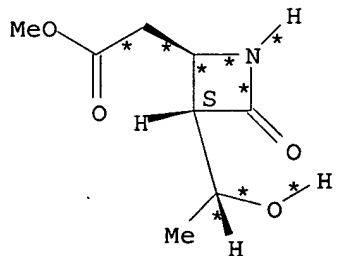
● Na⁺



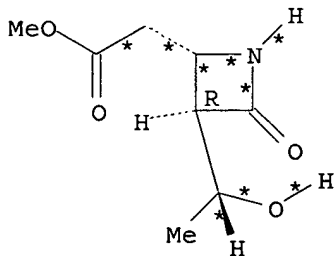
2 R

● Na⁺

8
STEPS
→



AJ
YIELD 95%(61)



AK
YIELD 95%(39)

RX(16) RCT AY 814-68-6
RGT AZ 26628-22-8 NaN₃

PRO A 50830-56-3
 SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
 RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
 PRO C 84713-20-2
 SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)
 RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8 Et₃N
 SOL 109-99-9 THF

STAGE(2)
 RCT R 122313-67-1
 SOL 109-99-9 THF

STAGE(3)
 RGT K 67-56-1 MeOH, U 630-08-0 CO
 SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
 RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
 PRO AA 122313-70-6, AB 122313-71-7
 SOL 67-56-1 MeOH
 NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
 RGT J 1333-74-0 H₂
 PRO AC 122313-59-1, AD 122313-60-4
 CAT 7440-05-3 Pd
 SOL 67-56-1 MeOH
 NTE 94% overall

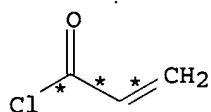
RX(9) RCT AC 122313-59-1, AD 122313-60-4
 RGT Z 538-75-0 DCC
 PRO AE 122313-61-5, AF 122313-62-6
 SOL 109-99-9 THF

RX(10) RCT AE 122313-61-5
 RGT AH 24057-28-1 Pyridinium tosylate
 PRO AG 122313-63-7
 SOL 67-64-1 Me₂CO

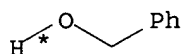
RX(11) RCT AG 122313-63-7
 RGT AL 54575-49-4 K Selectride
 PRO AJ 106248-39-9, AK 86421-11-6
 SOL 109-99-9 THF

RX(98) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
 RX(13), RX(14)

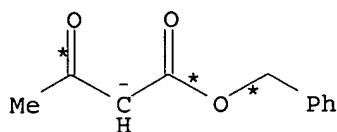
RX(98) 2 AY + 2 B + 2 R + 2 AQ ==> 2
 AV



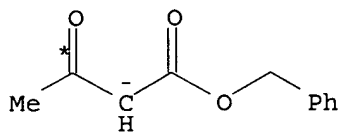
2 AY



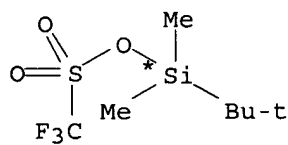
2 B

● Na⁺

R

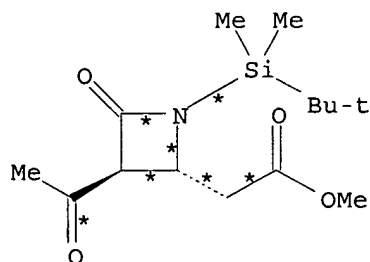
● Na⁺

R

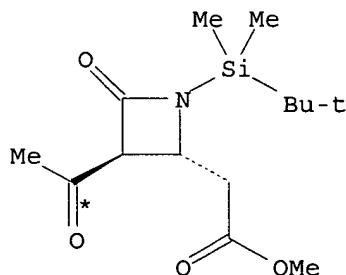


2 AQ

8
STEPS
→



AV
YIELD 100%



AV
YIELD 100%

RX(16) RCT AY 814-68-6
RGT AZ 26628-22-8 NaN₃
PRO A 50830-56-3
SOL 108-88-3 PhMe, 7732-18-5 Water

RX(1) RCT A 50830-56-3, B 100-51-6
RGT D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
PRO C 84713-20-2
SOL 108-88-3 PhMe

RX(5) RCT C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8

Et3N
SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)3, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H2
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

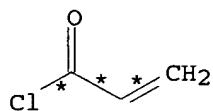
RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine
PRO AR 122313-64-8, AS 122313-65-9
SOL 75-09-2 CH2Cl2

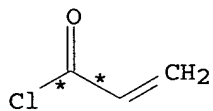
RX(14) RCT AR 122313-64-8, AS 122313-65-9
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV 122332-75-6
SOL 67-64-1 Me2CO

RX(100) OF 100 COMPOSED OF RX(16), RX(1), RX(5), RX(19), RX(8), RX(9),
RX(13), RX(14), RX(15)

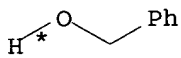
RX(100) 3 AY + 3 B + 3 R + 3 AQ ==>
AW + AX



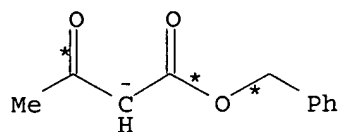
2 AY



AY

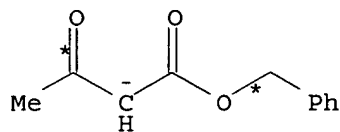


3 B



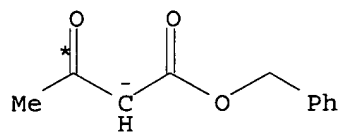
● Na⁺

R



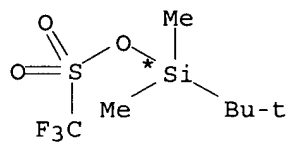
● Na⁺

R



● Na⁺

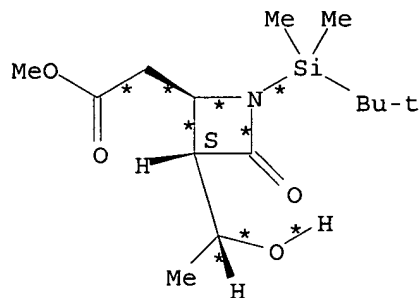
R



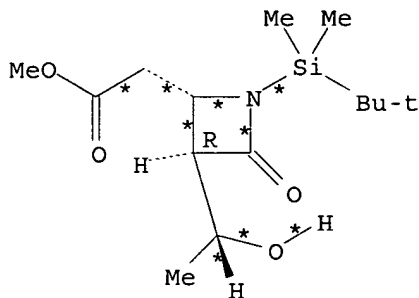
3 AQ

9

STEPS
→



AW
YIELD 86% (50)



AX
YIELD 86% (50)

RX(16)	RCT	AY 814-68-6
	RGT	AZ 26628-22-8 NaN ₃
	PRO	A 50830-56-3
	SOL	108-88-3 PhMe, 7732-18-5 Water
RX(1)	RCT	A 50830-56-3, B 100-51-6
	RGT	D 123-31-9 Hydroquinone, E 110-86-1 Pyridine
	PRO	C 84713-20-2
	SOL	108-88-3 PhMe
RX(5)	RCT	C 84713-20-2

STAGE(1)

RGT H 14592-56-4 PdCl₂(MeCN)₂, I 121-44-8
Et₃N
SOL 109-99-9 THF

STAGE(2)

RCT R 122313-67-1
SOL 109-99-9 THF

STAGE(3)

RGT K 67-56-1 MeOH, U 630-08-0 CO
SOL 109-99-9 THF, 67-56-1 MeOH

PRO S 122313-55-7, T 122313-56-8

RX(19) RCT S 122313-55-7, T 122313-56-8
RGT BC 149-73-5 CH(OMe)₃, BD 104-15-4 TsOH
PRO AA 122313-70-6, AB 122313-71-7
SOL 67-56-1 MeOH
NTE 90% overall

RX(8) RCT AA 122313-70-6, AB 122313-71-7
RGT J 1333-74-0 H₂
PRO AC 122313-59-1, AD 122313-60-4
CAT 7440-05-3 Pd
SOL 67-56-1 MeOH
NTE 94% overall

RX(9) RCT AC 122313-59-1, AD 122313-60-4
RGT Z 538-75-0 DCC
PRO AE 122313-61-5, AF 122313-62-6
SOL 109-99-9 THF

RX(13) RCT AE 122313-61-5, AF 122313-62-6, AQ 69739-34-0
RGT AT 108-48-5 2,6-Lutidine
PRO AR 122313-64-8, AS 122313-65-9
SOL 75-09-2 CH₂Cl₂

RX(14) RCT AR 122313-64-8, AS 122313-65-9
RGT AH 24057-28-1 Pyridinium tosylate
PRO AV 122332-75-6
SOL 67-64-1 Me₂CO

RX(15) RCT AV 122332-75-6
RGT AL 54575-49-4 K Selectride
PRO AW 122313-66-0, AX 122405-37-2
SOL 109-99-9 THF

L20 ANSWER 6 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 109:170611 CASREACT

TITLE: Diversity in modes of reactions of
[η³-1-(trimethylsiloxy)allyl]iron
dicarbonyl nitronyl complexes. Nucleophilic
addition and cyclization of the allylic
ligands

AUTHOR(S): Ito, Keiji; Nakanishi, Saburo; Otsuji, Yoshio

CORPORATE SOURCE: Dep. Ind. Chem., Osaka Prefect. Coll.

Technol., Osaka, 572, Japan

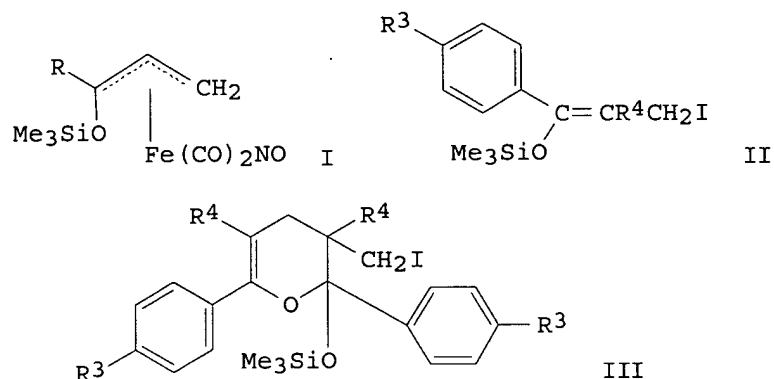
SOURCE: Chemistry Letters (1988), (3), 473-6

CODEN: CMLTAG; ISSN: 0366-7022

DOCUMENT TYPE:
LANGUAGE:
CLASSIFICATION:

Journal
English
29-12 (Organometallic and Organometalloidal
Compounds)
Section cross-reference(s): 23, 25, 27

GRAPHIC IMAGE:



ABSTRACT:

The title iron complexes (I; R = Ph, Et, OMe) derived from $\text{Me}_3\text{SiOCR:CHCH}_2\text{I}$ and $[\text{Bu}_4\text{N}][\text{Fe}(\text{CO})_3\text{NO}]$ reacted with carbon nucleophiles such as $\text{NaCH}(\text{CO}_2\text{Et})_2$ to give $\text{RCOCH}_2\text{CH}_2\text{CHR}_1\text{R}_2$ (same R; $\text{R}_1 = \text{R}_2 = \text{CO}_2\text{Et}$, cyano; $\text{R}_1 = \text{Ac}$, $\text{R}_2 = \text{CO}_2\text{Et}$) in 42-95% yields. The addition occurred at the 3-position of the ligands with high regioselectivity. However, the iron complexes derived from 2-alkyl-3-iodo-1-trimethylsiloxypropenes II ($\text{R}_3 = \text{H, Me, OMe, Cl}$; $\text{R}_4 = \text{Me, Et}$) underwent cyclization reaction with the same siloxypropenes to give dihydropyran derivs. III.

SUPPL. TERM: methylsiloxyallyliron dicarbonyl nitrosyl complex
addn; cyclization allylic ligand; pyran
siloxyiodomethylphenyl; iron complex addn
nucleophile regiochem

INDEX TERM: Regiochemistry
(of addition reaction of iodosiloxypropenes with
carbonylnitrosoiron complex)

INDEX TERM: Addition reaction
(of iodosiloxypropenes with carbonylnitrosoiron
complex)

INDEX TERM: 96206-23-4
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with iodosilyloxypropenes)

INDEX TERM: 670-80-4 996-82-7 20334-42-3 34284-28-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with iron complexes)

INDEX TERM: 116309-64-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with nucleophiles)

INDEX TERM: 96-33-3, Methyl acrylate 768-03-6, Phenyl vinyl
ketone 769-60-8 1629-58-9, Ethyl vinyl ketone
6230-72-4 6230-73-5 22731-65-3 62834-89-3
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(iodosilylation of)

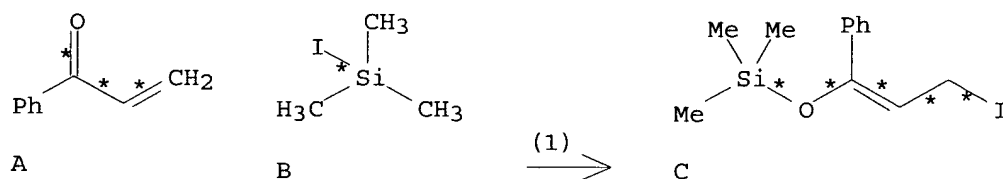
INDEX TERM: 116981-02-3P 116981-03-4P 116981-04-5P
 116981-05-6P 116981-06-7P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and addition reaction of, with iron
 complexes)

INDEX TERM: 116309-63-8P 116309-67-2P 117008-24-9P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and addition reaction of, with nucleophiles)

INDEX TERM: 108162-05-6P 108162-06-7P 116385-36-5P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with iron complex)

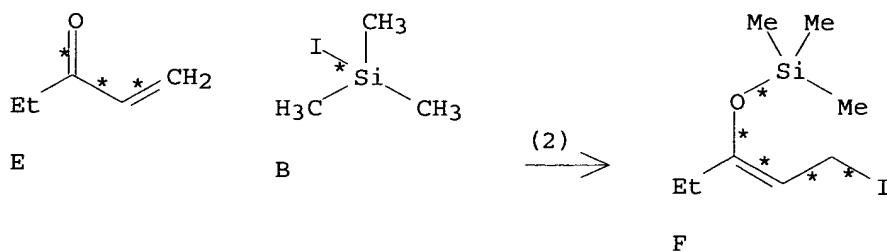
INDEX TERM: 3709-23-7P 5331-68-0P 10407-33-7P 22274-75-5P
 70431-98-0P 72357-49-4P 111372-86-2P
 116981-00-1P 116981-01-2P 116981-07-8P
 116981-08-9P 116981-09-0P 116981-10-3P
 116981-11-4P 116994-60-6P
 ROLE: SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation of)

RX(1) OF 50 A + B ==> C...



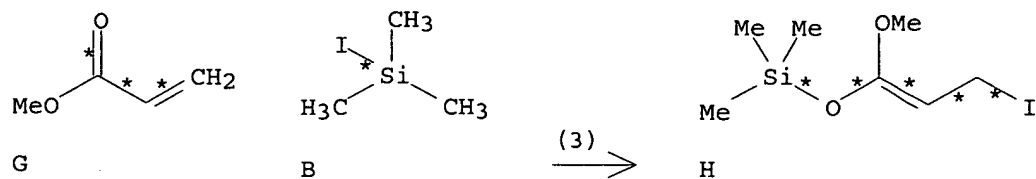
RX(1) RCT A 768-03-6, B 16029-98-4
 PRO C 116385-36-5
 SOL 75-09-2 CH₂Cl₂

RX(2) OF 50 E + B ==> F...



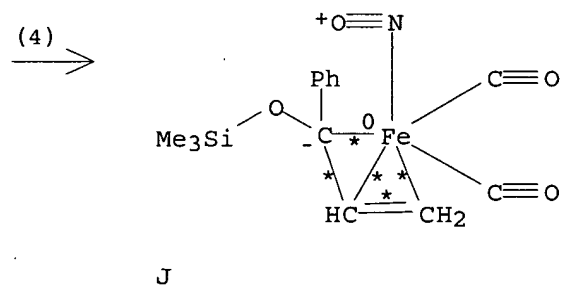
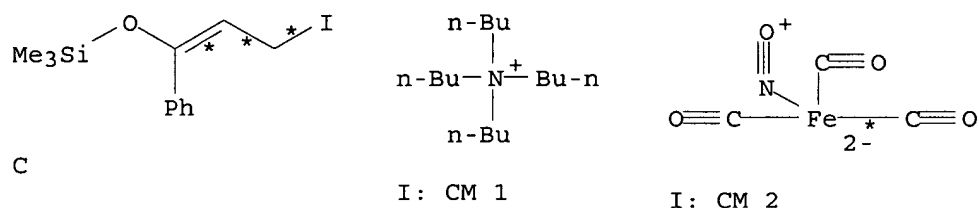
RX(2) RCT E 1629-58-9, B 16029-98-4
 PRO F 108162-05-6
 SOL 75-09-2 CH₂Cl₂

RX(3) OF 50 G + B ==> H...



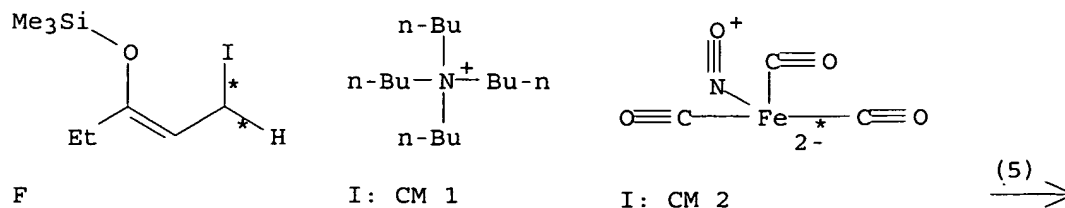
RX(3) RCT G 96-33-3, B 16029-98-4
 PRO H 108162-06-7
 SOL 75-09-2 CH₂Cl₂

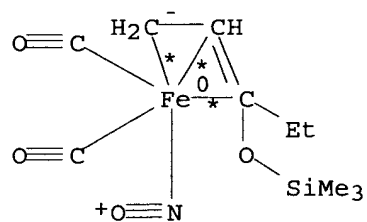
RX(4) OF 50 ...C + I ==> J...



RX(4) RCT C 116385-36-5, I 96206-23-4
 PRO J 116309-67-2
 SOL 75-09-2 CH₂Cl₂

RX(5) OF 50 ...F + I ==> K...

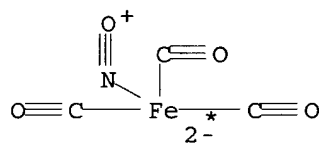
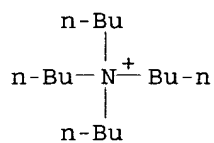
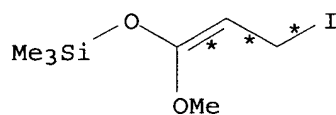




K

RX(5) RCT F 108162-05-6, I 96206-23-4
 PRO K 116309-63-8
 SOL 75-09-2 CH2Cl2

RX(6) OF 50 ...H + I ==> L...

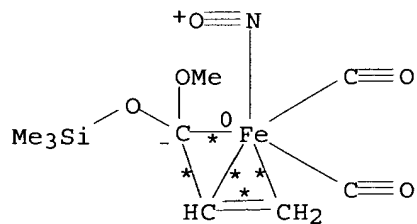


H

I: CM 1

I: CM 2

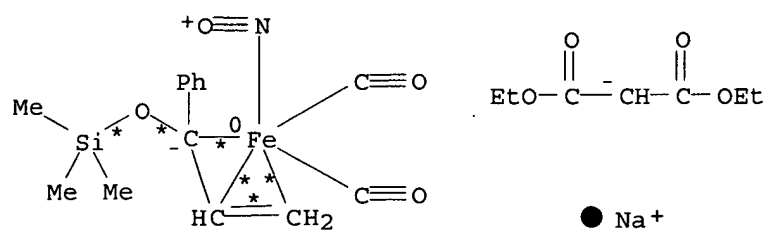
(6) →



L

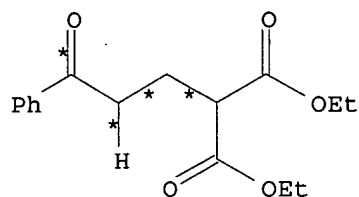
RX(6) RCT H 108162-06-7, I 96206-23-4
 PRO L 117008-24-9
 SOL 75-09-2 CH2Cl2

RX(7) OF 50 ...J + M ==> N



J

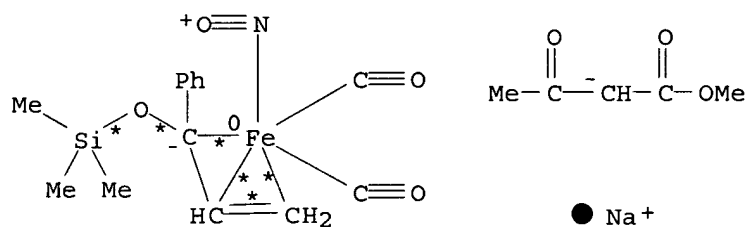
M

(7) \longrightarrow 

N
YIELD 95%

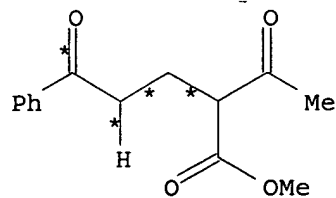
RX (7) RCT J 116309-67-2, M 996-82-7
PRO N 3709-23-7
SOL 75-09-2 CH₂Cl₂

RX (8) OF 50 ...J + O ==> P



J

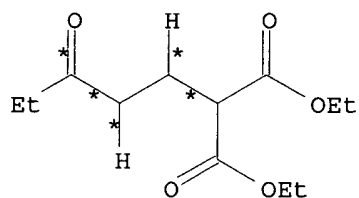
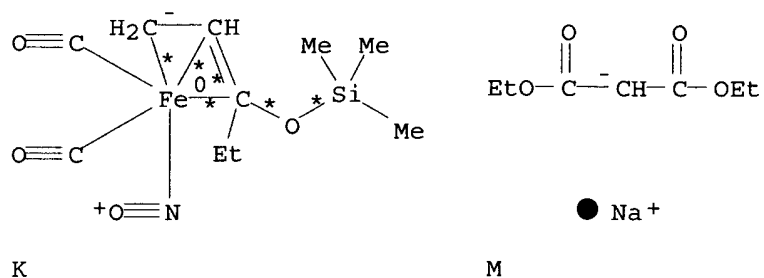
O

(8) \longrightarrow 

P
YIELD 42%

RX(8) RCT J 116309-67-2, O 34284-28-1
 PRO P 116981-00-1
 SOL 75-09-2 CH₂Cl₂

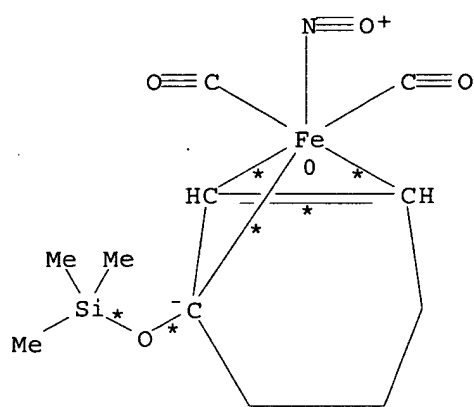
RX(9) OF 50 ...K + M ==> Q



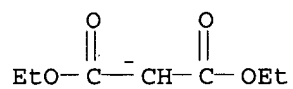
Q
 YIELD 75%

RX(9) RCT K 116309-63-8, M 996-82-7
 PRO Q 70431-98-0
 SOL 75-09-2 CH₂Cl₂

RX(10) OF 50 R + M ==> S

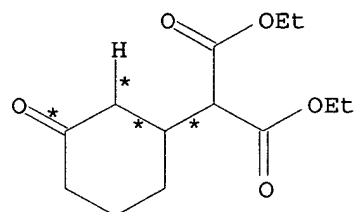


R

● Na⁺

M

(10) →

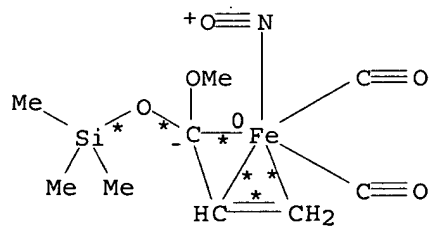


S

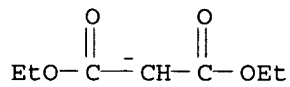
YIELD 90%

RX(10) RCT R 116309-64-9, M 996-82-7
 PRO S 22274-75-5
 SOL 75-09-2 CH₂Cl₂

RX(11) OF 50 ...L + M ==> T

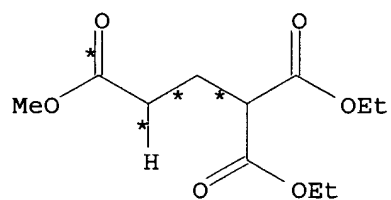


L

● Na⁺

M

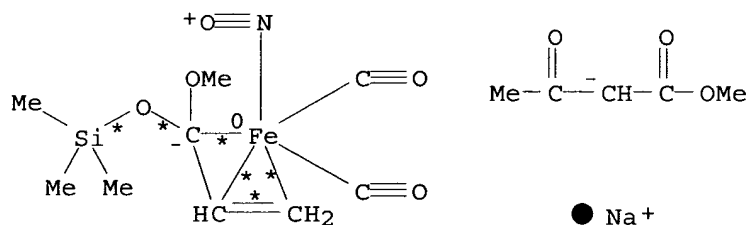
(11) →



T
YIELD 95%

RX(11) RCT L 117008-24-9, M 996-82-7
PRO T 5331-68-0
SOL 75-09-2 CH2Cl2

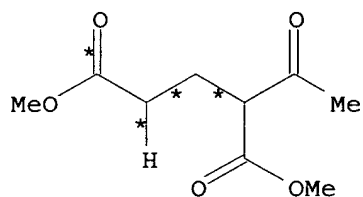
RX(12) OF 50 ...L + O ==> U



L

O

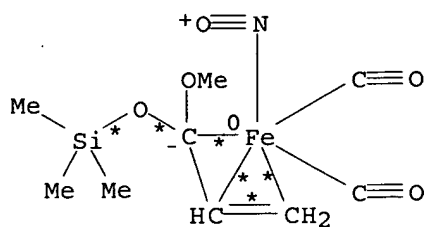
(12) →



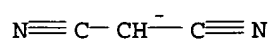
U
YIELD 60%

RX(12) RCT L 117008-24-9, O 34284-28-1
PRO U 116981-01-2
SOL 75-09-2 CH2Cl2

RX(13) OF 50 ...L + V ==> W



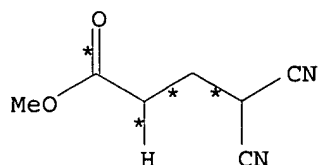
L



V



(13)

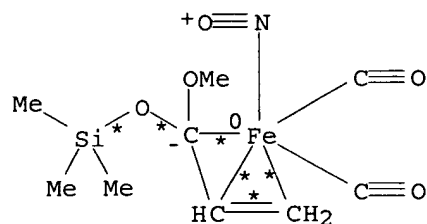


W

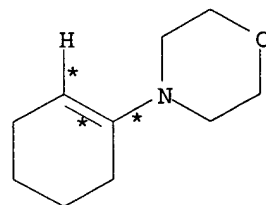
YIELD 92%

RX(13) RCT L 117008-24-9, V 20334-42-3
 PRO W 111372-86-2
 SOL 75-09-2 CH2Cl2

RX(14) OF 50 ...L + X ==> Y

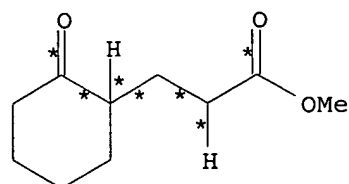


L



X

(14)

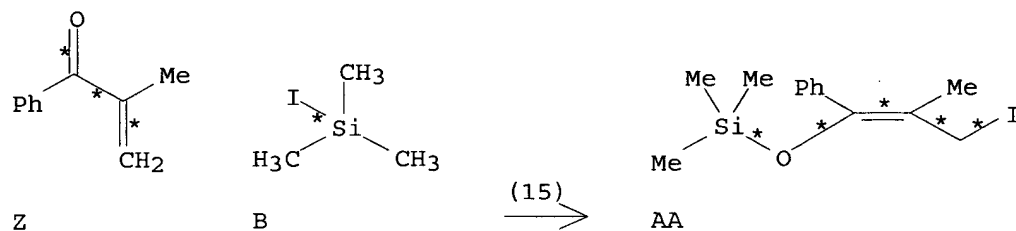


Y

YIELD 89%

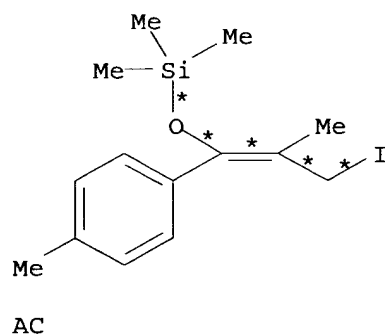
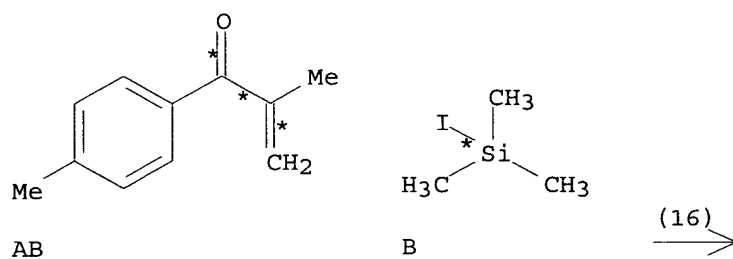
RX(14) RCT L 117008-24-9, X 670-80-4
 PRO Y 10407-33-7
 SOL 75-09-2 CH₂Cl₂

RX(15) OF 50 Z + B ==> AA...



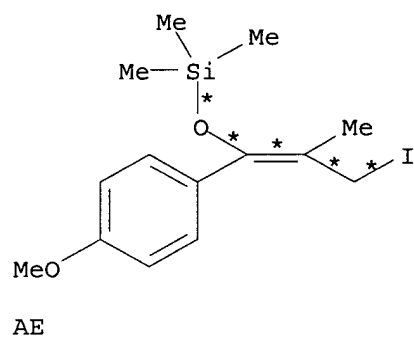
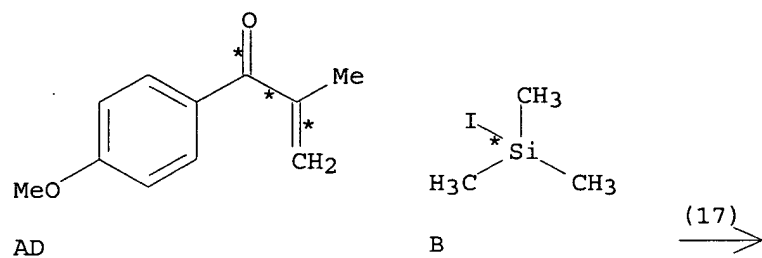
RX(15) RCT Z 769-60-8, B 16029-98-4
 PRO AA 116981-02-3
 SOL 75-09-2 CH₂Cl₂

RX(16) OF 50 AB + B ==> AC...



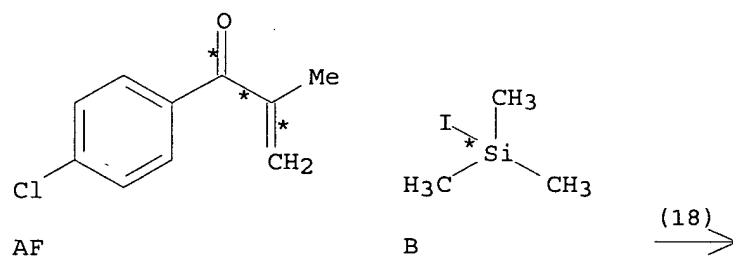
RX(16) RCT AB 62834-89-3, B 16029-98-4
 PRO AC 116981-03-4
 SOL 75-09-2 CH₂Cl₂

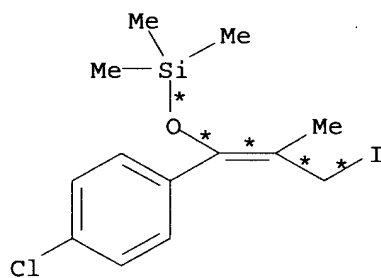
RX(17) OF 50 AD + B ==> AE...



RX(17) RCT AD 6230-72-4, B 16029-98-4
 PRO AE 116981-04-5
 SOL 75-09-2 CH₂Cl₂

RX(18) OF 50 AF + B ==> AG...

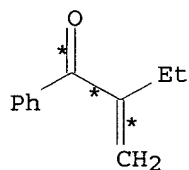




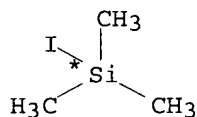
AG

RX(18) RCT AF 6230-73-5, B 16029-98-4
 PRO AG 116981-05-6
 SOL 75-09-2 CH2Cl2

RX(19) OF 50 AH + B ==> AI...

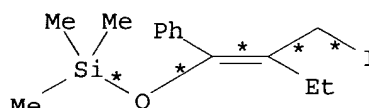


AH



B

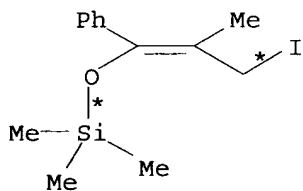
(19) >



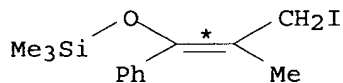
AI

RX(19) RCT AH 22731-65-3, B 16029-98-4
 PRO AI 116981-06-7
 SOL 75-09-2 CH2Cl2

RX(20) OF 50 ...2 AA ==> AJ

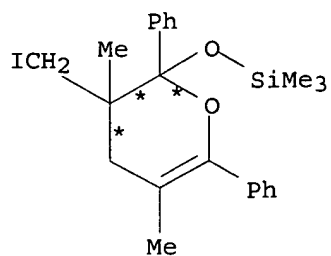


AA



AA

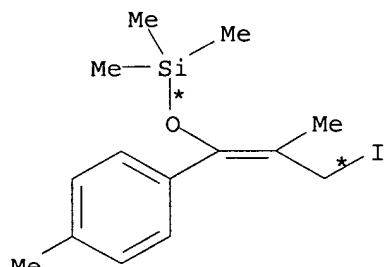
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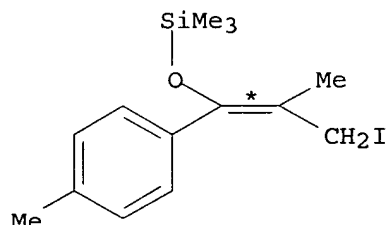
AJ

RX(20) RCT AA 116981-02-3
 RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-,
 (T-4)-tricarbonylnitrosylferrate(1-)
 PRO AJ 116981-07-8
 SOL 75-09-2 CH2Cl2

RX(21) OF 50 ...2 AC ==> AK

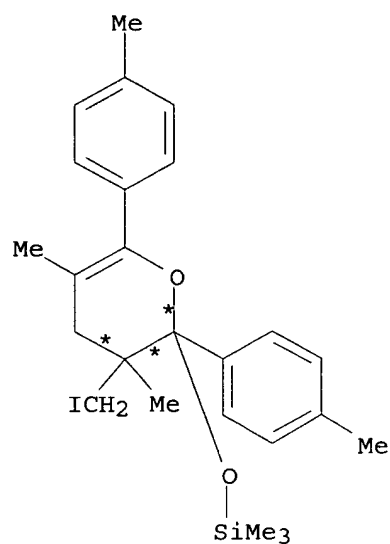


AC



AC

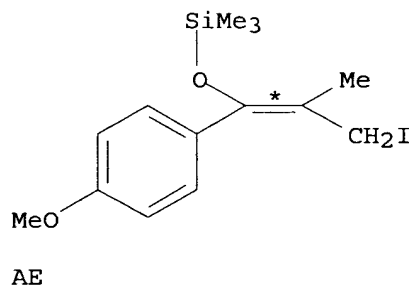
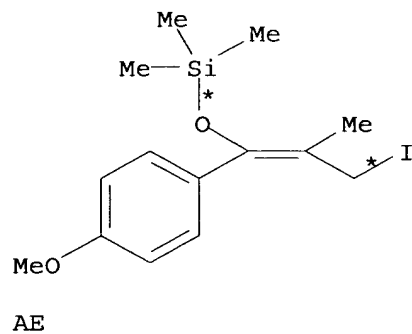
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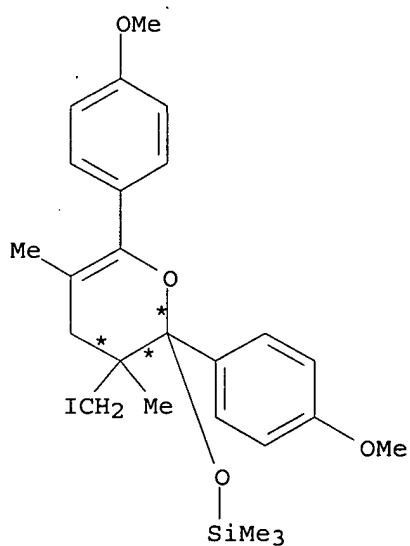
AK

RX(21) RCT AC 116981-03-4
 RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-,
 (T-4)-tricarboxylnitrosylferrate(1-)
 PRO AK 116981-08-9
 SOL 75-09-2 CH₂Cl₂

RX(22) OF 50 ...2 AE ==> AL



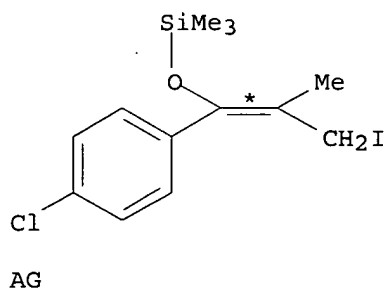
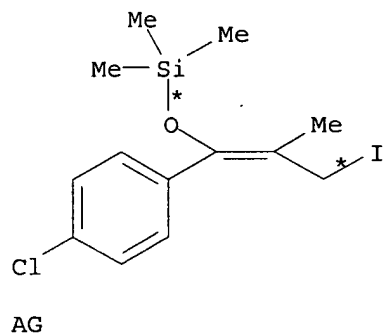
(22)
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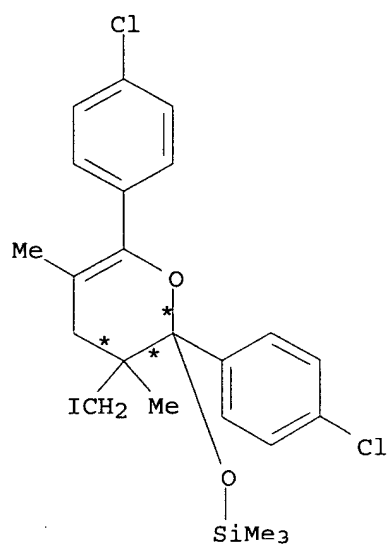
AL

RX(22) RCT AE 116981-04-5
 RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-,
 (T-4)-tricarbonylnitrosylferrate(1-)
 PRO AL 116981-09-0
 SOL 75-09-2 CH2Cl2

RX(23) OF 50 ...2 AG ==> AM



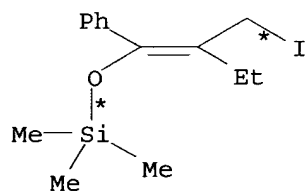
(23) →



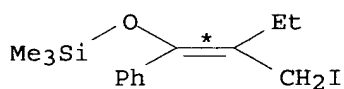
AM

RX (23) RCT AG 116981-05-6
 RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-,
 (T-4)-tricarboxylnitrosylferrate(1-)
 PRO AM 116981-10-3
 SOL 75-09-2 CH2Cl2

RX (24) OF 50 ...2 AI ==> AN

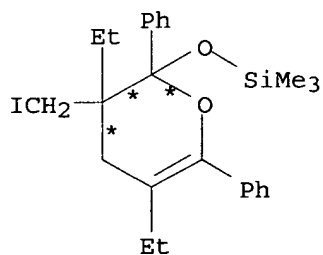


AI



AI

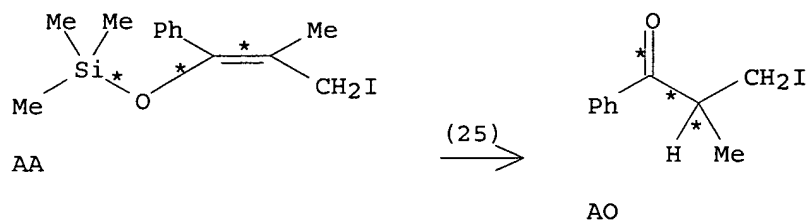
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AN

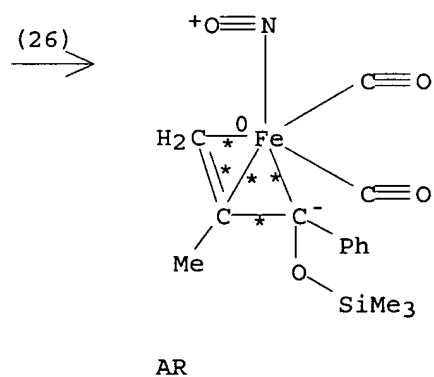
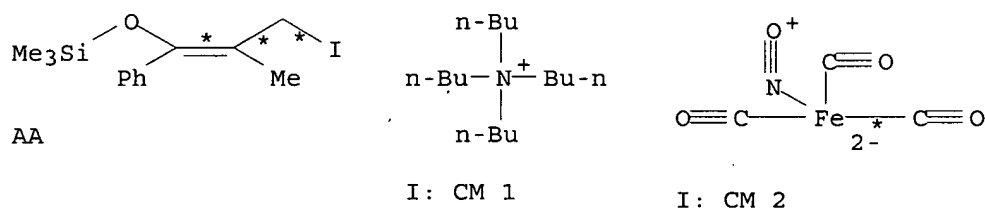
RX(24) RCT AI 116981-06-7
 RGT I 96206-23-4 1-Butanaminium, N,N,N-tributyl-,
 (T-4)-tricarbonylnitrosylferrate(1-)
 PRO AN 116981-11-4
 SOL 75-09-2 CH₂Cl₂

RX(25) OF 50 ...AA ==> AO



RX(25) RCT AA 116981-02-3
 RGT AP 7647-01-0 HCl
 PRO AO 72357-49-4
 SOL 7732-18-5 Water

RX(26) OF 50 ...AA + I ==> AR

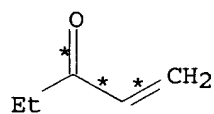


RX(26) RCT AA 116981-02-3, I 96206-23-4
 PRO AR 116994-60-6
 SOL 75-09-2 CH₂Cl₂

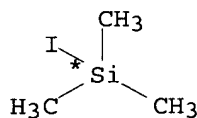
RX(46) OF 50 COMPOSED OF RX(2), RX(5), RX(9)

RX(46) E + B + I + M ==>

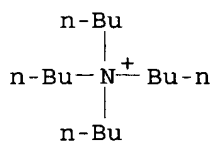
Q



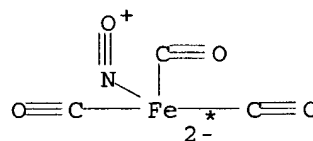
E



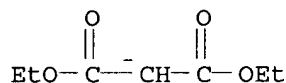
B



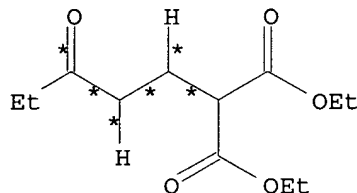
I: CM 1



I: CM 2



M

3
STEPS
→Q
YIELD 75%

RX(2) RCT E 1629-58-9, B 16029-98-4

PRO F 108162-05-6

SOL 75-09-2 CH2Cl2

RX(5) RCT F 108162-05-6, I 96206-23-4

PRO K 116309-63-8

SOL 75-09-2 CH2Cl2

RX(9) RCT K 116309-63-8, M 996-82-7

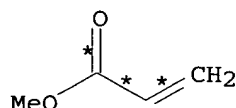
PRO Q 70431-98-0

SOL 75-09-2 CH2Cl2

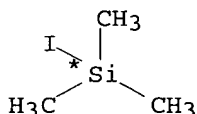
RX(47) OF 50 COMPOSED OF RX(3), RX(6), RX(11)

RX(47) G + B + I + M ==>

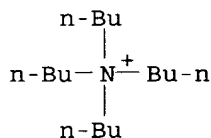
T



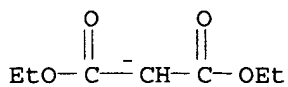
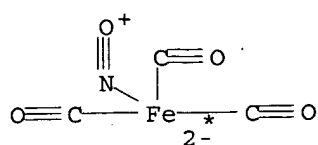
G



B



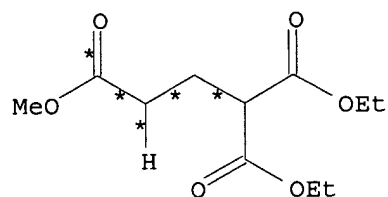
I: CM 1



I: CM 2

● Na⁺3
STEPS
→

M

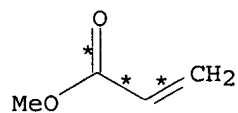
T
YIELD 95%

RX(3) RCT G 96-33-3, B 16029-98-4
 PRO H 108162-06-7
 SOL 75-09-2 CH2Cl2

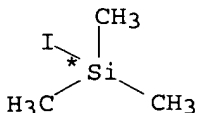
RX(6) RCT H 108162-06-7, I 96206-23-4
 PRO L 117008-24-9
 SOL 75-09-2 CH2Cl2

RX(11) RCT L 117008-24-9, M 996-82-7
 PRO T 5331-68-0
 SOL 75-09-2 CH2Cl2

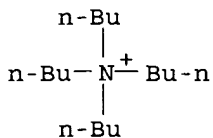
RX(48) OF 50 COMPOSED OF RX(3), RX(6), RX(12)
 RX(48) G + B + I + O ==>
 U



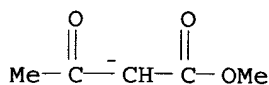
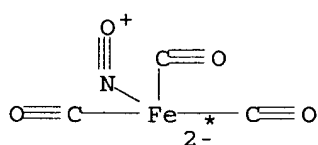
G



B



I: CM 1



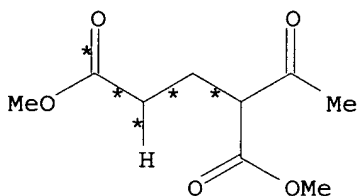
I: CM 2

● Na⁺

3

STEPS
→

O



U
YIELD 60%

RX(3) RCT G 96-33-3, B 16029-98-4
PRO H 108162-06-7
SOL 75-09-2 CH2Cl2

RX(6) RCT H 108162-06-7, I 96206-23-4
PRO L 117008-24-9
SOL 75-09-2 CH2Cl2

RX(12) RCT L 117008-24-9, O 34284-28-1
PRO U 116981-01-2
SOL 75-09-2 CH2Cl2

L20 ANSWER 7 OF 7 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 106:137899 CASREACT

TITLE: Synthesis of functionalized 1,4-dienes by
addition of functionalized allylzinc compounds
to alkynes and their cyclization to
heterocycles and carbocycles

AUTHOR(S): Knochel, P.; Normant, J. F.

CORPORATE SOURCE: Lab. Chim. Org. Elem., Univ. P. M. Curie,
Paris, 75230/05, Fr.

SOURCE: Journal of Organometallic Chemistry (1986),
309(1-2), 1-23

CODEN: JORCAI; ISSN: 0022-328X

DOCUMENT TYPE: Journal

LANGUAGE: French

CLASSIFICATION: 23-3 (Aliphatic Compounds)

Section cross-reference(s): 27, 28

ABSTRACT:

The regiospecific addition of functionalized allylic bromides to terminal alkynes in the presence of zinc furnishes a great variety of highly functionalized 1,4-dienes with moderate to good yields. The synthetic utility of these 1,4-dienes is demonstrated by various cyclization

reactions leading to an α -methylene- γ -butyrolactone, to 3,5-difunctionalized piperidines, to a cyclic triester and to 6- or 7-membered phosphorus heterocyclic compds.

SUPPL. TERM: allyl bromide addn alkyne zinc; piperidine;
oxaphosphorinane oxo alkoxy

INDEX TERM: Allylic compounds
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(bromides, functionalized, addition reaction of,
with terminal alkynes and zinc)

INDEX TERM: Addition reaction
(of functionalized allyl bromides with terminal
alkynes and zinc)

INDEX TERM: Alkynes
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(α -, addition reaction of, with functionalized
allyl bromides and zinc)

INDEX TERM: 122-52-1, Triethyl phosphite
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Arbuzov reaction of, with methylene bromide)

INDEX TERM: 74-95-3, Methylene bromide
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(Arbuzov reaction of, with tri-Et phosphite)

INDEX TERM: 75-36-5, Acetyl chloride
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(acylation by, of allyl silyl ethers)

INDEX TERM: 627-09-8 629-05-0, 1-Octyne 5651-88-7, Phenyl
propargyl sulfide 13361-64-3,
Propargyltrimethylsilane 13397-78-9 17869-76-0
18938-38-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with functionalized allyl
bromide derivative and zinc)

INDEX TERM: 693-02-7, 1-Hexyne 5582-62-7, Propargyl
trimethylsilyl ether 16314-18-4 17869-75-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with functionalized allyl
bromides and zinc)

INDEX TERM: 62097-05-6
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(addition reaction of, with propargyl silyl ether
derivative and zinc)

INDEX TERM: 123-75-1, Pyrrolidine, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(amidation by, of dibromoisobutyric acid)

INDEX TERM: 63164-16-9
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(amidation of, by pyrrolidine)

INDEX TERM: 38281-98-0
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(bromination of)

INDEX TERM: 55287-89-3
ROLE: PROC (Process)
(conversion of, to allyl bromide analog)

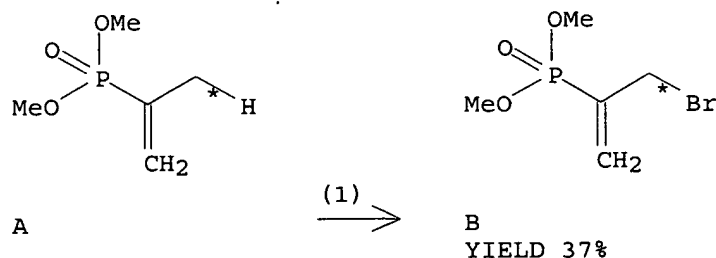
INDEX TERM: 37850-75-2
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(conversion of, to dibromoisopropyl sulfoxide
derivative)

INDEX TERM: 111-68-2, 1-Heptylamine
ROLE: RCT (Reactant); RACT (Reactant or reagent)

(cycloaddn. reaction of, with pentadiene derivative)
INDEX TERM: 100-46-9, Benzylamine, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn. reaction of, with pentadienes)
INDEX TERM: 105-53-3, Diethyl malonate
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(cycloaddn.-cyclocondensation of, with pentenyl
acetate derivative)
INDEX TERM: 115-11-7, Isobutylene, reactions
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(esterification by, of bromoacetic acid)
INDEX TERM: 79-08-3, Bromoacetic acid
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(esterification of)
INDEX TERM: 107345-39-1P
ROLE: FORM (Formation, nonpreparative); PREP
(Preparation)
(formation of, in addition reaction of
carbalkoxyallyl bromide with alkynes and zinc)
INDEX TERM: 107345-41-5P
ROLE: FORM (Formation, nonpreparative); PREP
(Preparation)
(formation of, in attempted addition reaction of
allyl bromide derivative with hexyne and zinc)
INDEX TERM: 1125-99-1
ROLE: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis of, and alkylation of product with
pentenyl acetate derivative)
INDEX TERM: 91476-12-9P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and acetylation of)
INDEX TERM: 107345-23-3P 107345-24-4P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with propargyl
silyl ether derivative and zinc)
INDEX TERM: 17435-72-2P 53913-96-5P 84308-48-5P
91445-18-0P 91476-10-7P 97147-24-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and addition reaction of, with terminal
alkynes and zinc)
INDEX TERM: 1660-94-2P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and conversion, to isopropenylphosphonic
acid derivative)
INDEX TERM: 91476-26-5P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with amines)
INDEX TERM: 107345-42-6P
ROLE: RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation and cycloaddn. reaction of, with
benzylamine)
INDEX TERM: 91476-21-0P 91476-22-1P 91476-23-2P
91476-24-3P
ROLE: RCT (Reactant); SPN (Synthetic preparation);

PREP (Preparation); RACT (Reactant or reagent)
 (preparation and cyclocondensation reaction of)
 INDEX TERM: 5292-43-3P, 1,1-Dimethylethyl bromoacetate
 ROLE: SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation and cyclocondensation with alkyne and
 zinc)
 INDEX TERM: 107345-37-9P 107345-38-0P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and dehydrobromination of)
 INDEX TERM: 91476-11-8P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and iodolactonization of)
 INDEX TERM: 93032-43-0P
 ROLE: RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and reaction of, with phosphorus
 tribromide)
 INDEX TERM: 91476-13-0P 91476-14-1P 91476-15-2P
 91476-16-3P 91476-17-4P 91476-18-5P
 91476-19-6P 91476-20-9P 91476-25-4P
 91476-27-6P 91476-28-7P 91476-29-8P
 91476-30-1P 91476-31-2P 91476-32-3P
 91476-33-4P 94225-07-7P 94225-08-8P
 94225-09-9P 97779-25-4P 97779-26-5P
 97779-27-6P 107345-25-5P 107345-26-6P
 107345-27-7P 107345-28-8P 107345-29-9P
 107345-30-2P 107345-31-3P 107345-32-4P
 107345-33-5P 107345-34-6P 107345-35-7P
 107345-36-8P 107345-40-4P 107345-43-7P
 107345-44-8P 107345-45-9P
 ROLE: SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation of)
 INDEX TERM: 50-00-0, Formaldehyde, reactions
 ROLE: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with methylenebisphosphonic acid
 derivative)

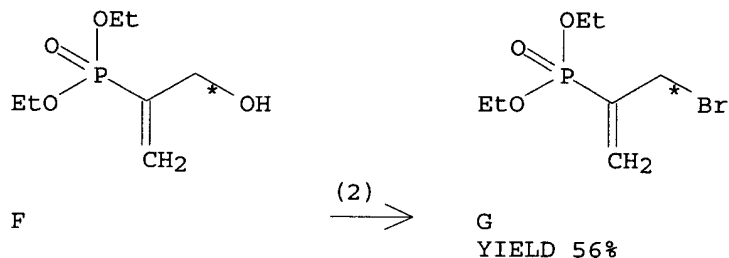
RX(1) OF 130 A ==> B...



RX(1) RCT A 38281-98-0
 RGT C 128-08-5 Bromosuccinimide, D 78-67-1 AIBN
 PRO B 84308-48-5

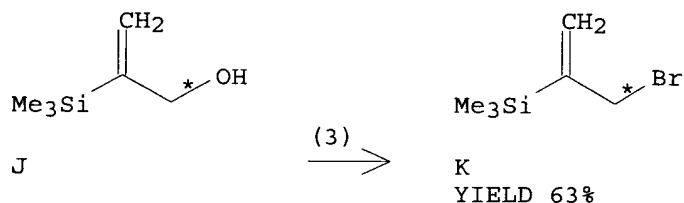
SOL 56-23-5 CCl4

RX(2) OF 130 ...F ==> G...



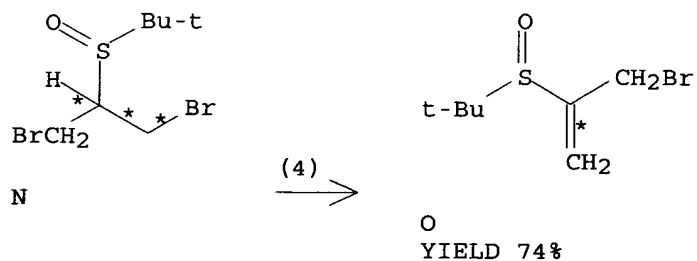
RX(2) RCT F 93032-43-0
 RGT H 7789-60-8 PBr3
 PRO G 91476-10-7
 SOL 60-29-7 Et2O

RX(3) OF 130 J ==> K...



RX(3) RCT J 55287-89-3
 RGT C 128-08-5 Bromosuccinimide, L 75-18-3 Me2S
 PRO K 91445-18-0
 SOL 75-09-2 CH2Cl2

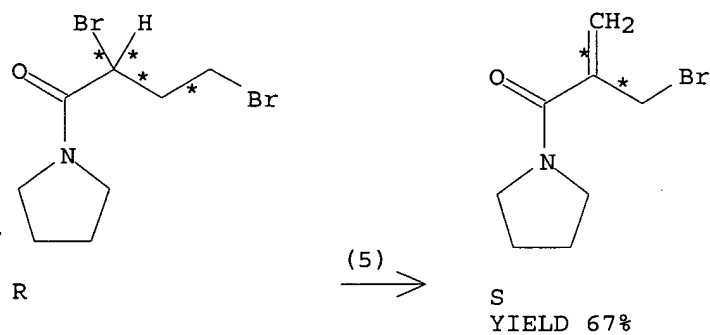
RX(4) OF 130 ...N ==> O...



RX(4) RCT N 107345-37-9
 RGT P 6674-22-2 DBU, Q 123-31-9 Hydroquinone

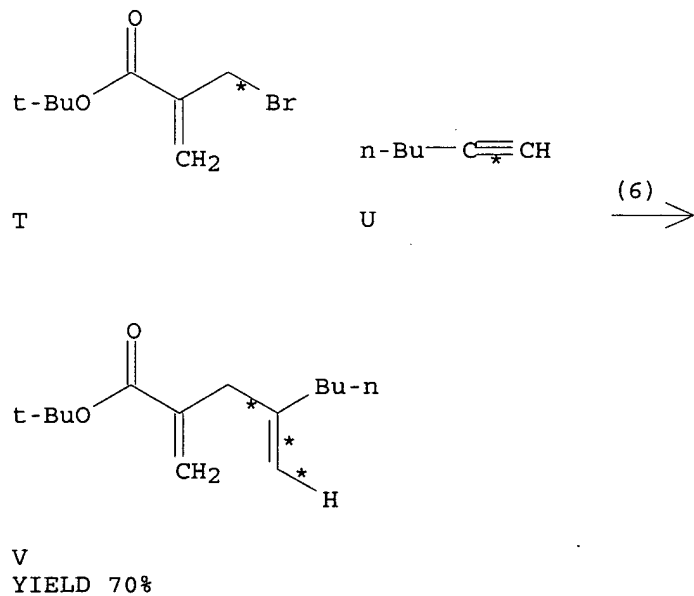
PRO O 107345-23-3
SOL 75-09-2 CH₂Cl₂

RX(5) OF 130 ...R ==> S...



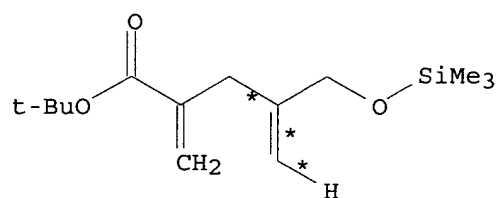
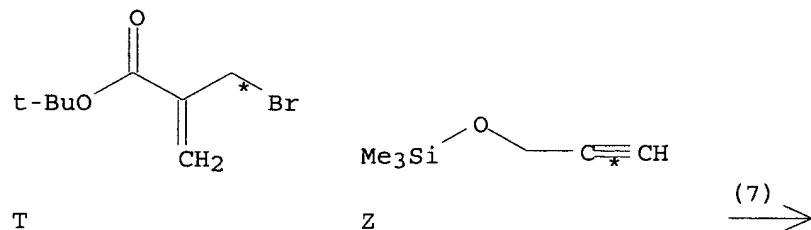
RX(5) RCT R 107345-38-0
 RGT P 6674-22-2 DBU, Q 123-31-9 Hydroquinone
 PRO S 107345-24-4
 SOL 75-09-2 CH₂Cl₂

RX(6) OF 130 T + U ==> V...



RX(6) RCT T 53913-96-5, U 693-02-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO V 91476-11-8
 SOL 109-99-9 THF

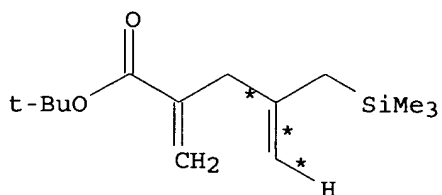
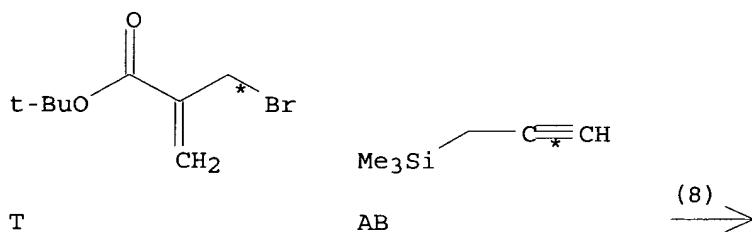
RX(7) OF 130 T + Z ==> AA...



AA
YIELD 81%

RX(7) RCT T 53913-96-5, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AA 91476-12-9
 SOL 109-99-9 THF

RX(8) OF 130 T + AB ==> AC

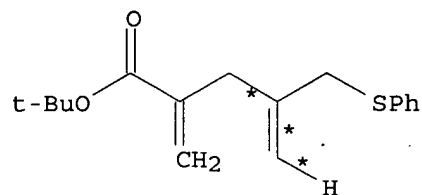
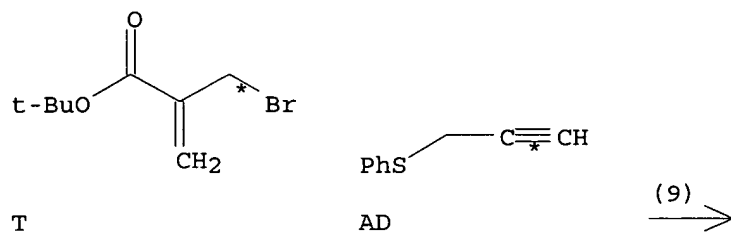


AC
YIELD 24%

RX(8) RCT T 53913-96-5, AB 13361-64-3

RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AC 107345-25-5
 SOL 109-99-9 THF

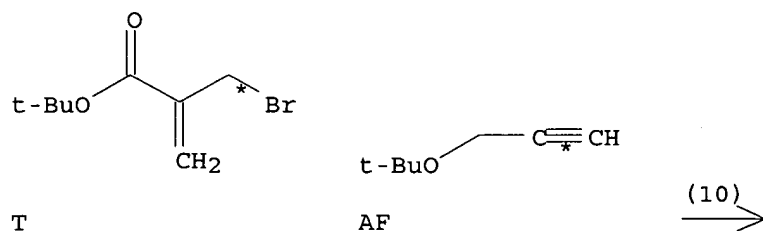
RX(9) OF 130 T + AD ==> AE

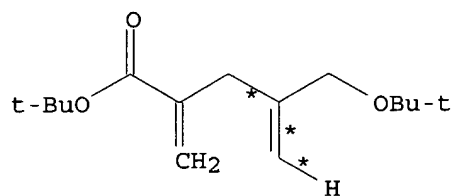


AE
 YIELD 55%

RX(9) RCT T 53913-96-5, AD 5651-88-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AE 91476-16-3
 SOL 109-99-9 THF

RX(10) OF 130 T + AF ==> AG

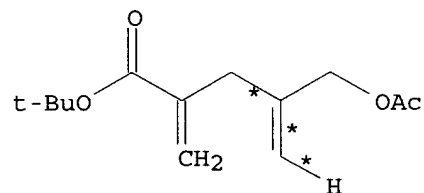
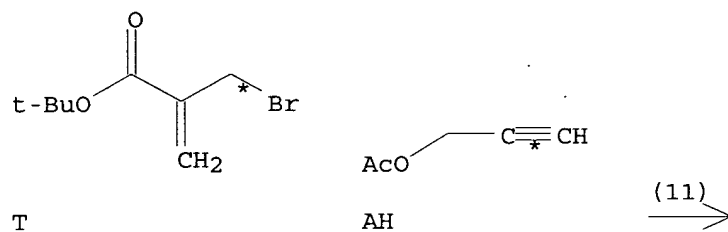




AG
YIELD 64%

RX(10) RCT T 53913-96-5, AF 16314-18-4
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AG 91476-14-1
SOL 109-99-9 THF

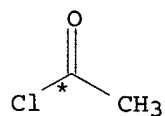
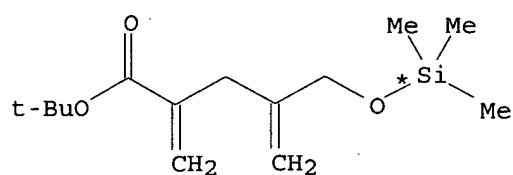
RX(11) OF 130 T + AH ==> AI...



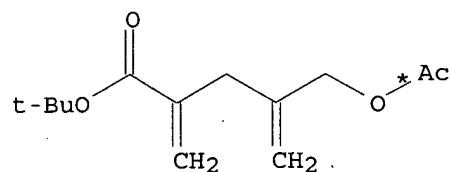
AI
YIELD 47%

RX(11) RCT T 53913-96-5, AH 627-09-8
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AI 91476-26-5
SOL 109-99-9 THF

RX(12) OF 130 ...AA + AJ ==> AI...



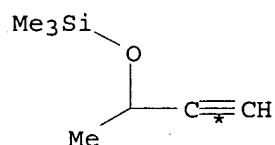
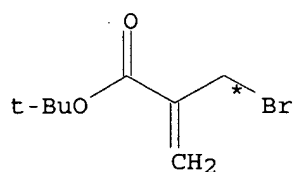
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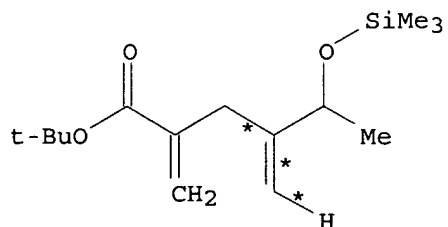
YIELD 88%

RX(12) RCT AA 91476-12-9, AJ 75-36-5
 RGT AK 64-19-7 AcOH
 PRO AI 91476-26-5
 SOL 60-29-7 Et2O, 64-19-7 AcOH

RX(13) OF 130 T + AL ==> AM



(13) →

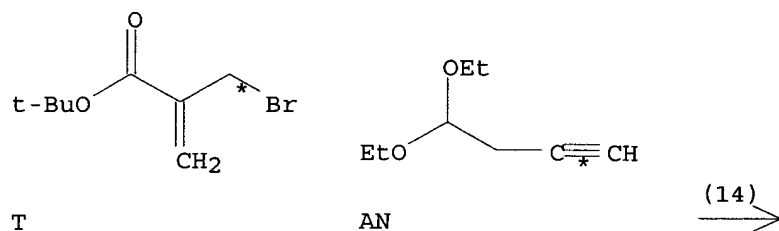


YIELD 54%

RX(13) RCT T 53913-96-5, AL 17869-76-0
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br

PRO AM 91476-15-2
SOL 109-99-9 THF

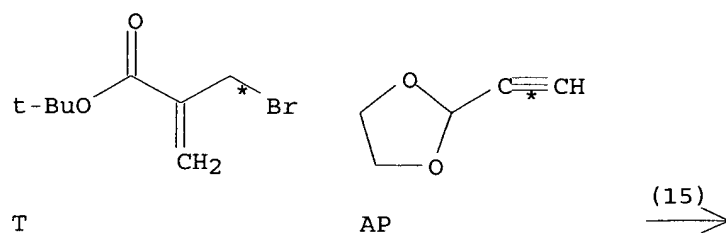
RX(14) OF 130 T + AN ==> AO

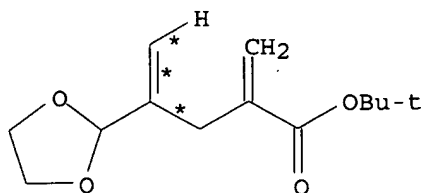


AO
YIELD 60%

RX(14) RCT T 53913-96-5, AN 13397-78-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AO 91476-17-4
SOL 109-99-9 THF

RX(15) OF 130 T + AP ==> AQ

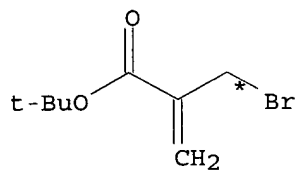




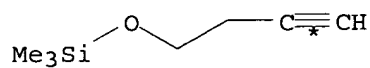
AQ
YIELD 28%

RX(15) RCT T 53913-96-5, AP 18938-38-0
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AQ 107345-26-6
SOL 109-99-9 THF

RX(16) OF 130 T + AR ==> AS

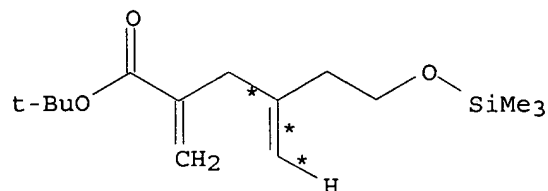


T



AR

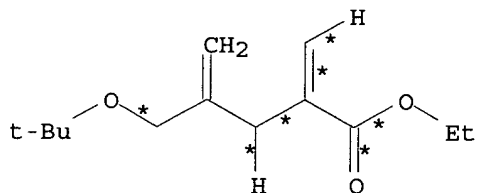
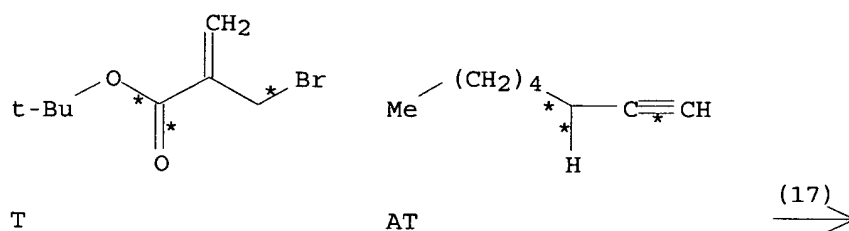
(16)
→



AS
YIELD 70%

RX(16) RCT T 53913-96-5, AR 17869-75-9
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AS 91476-13-0
SOL 109-99-9 THF

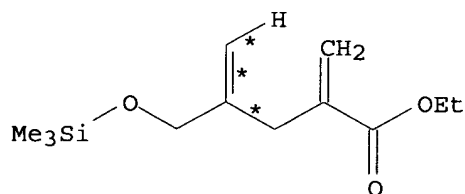
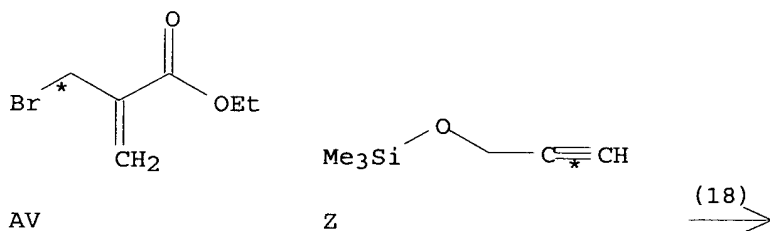
RX(17) OF 130 T + AT ==> AU



AU
YIELD 62%

RX(17) RCT T 53913-96-5, AT 629-05-0
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AU 91476-18-5
SOL 109-99-9 THF

RX (18) OF 130 AV + Z ==> AW

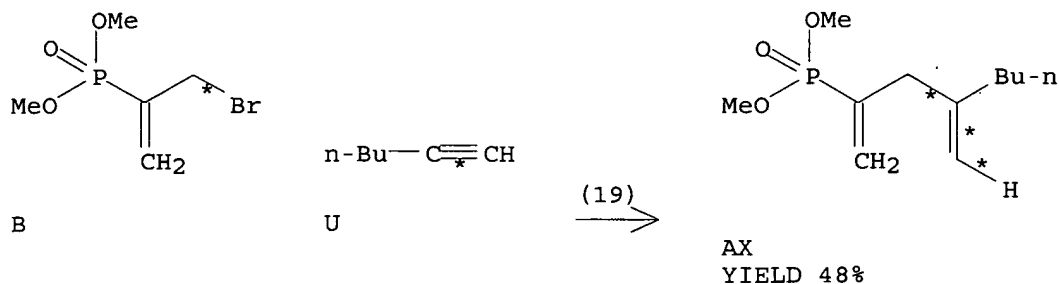


AW
YIELD 68%

RX(18) RCT AV 17435-72-2, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AW 91476-19-6

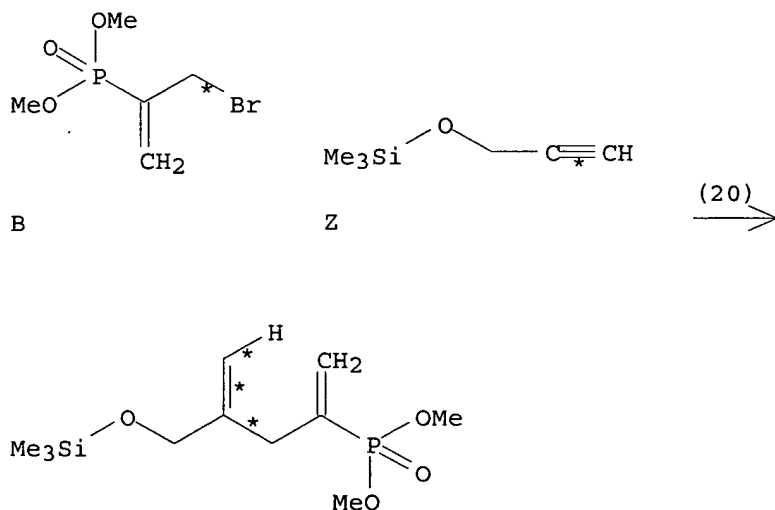
SOL 109-99-9 THF

RX(19) OF 130 ...B + U ==> AX



RX(19) RCT B 84308-48-5, U 693-02-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AX 91476-20-9
 SOL 109-99-9 THF

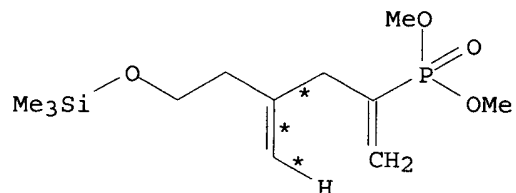
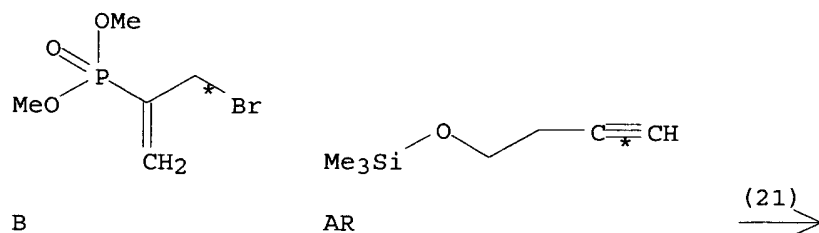
RX(20) OF 130 ...B + Z ==> AY...



AY

RX(20) RCT B 84308-48-5, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AY 107345-27-7
 SOL 109-99-9 THF

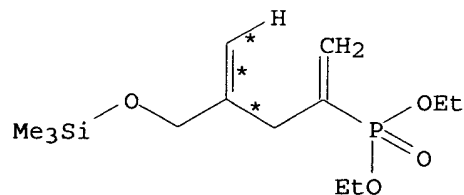
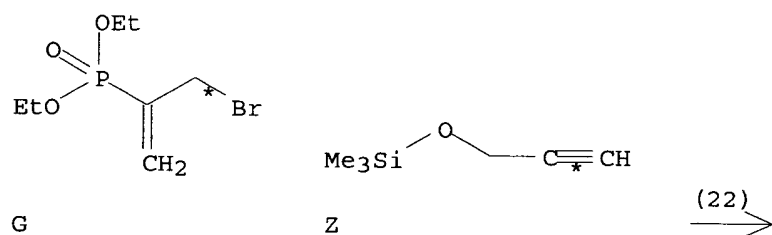
RX(21) OF 130 ...B + AR ==> AZ...



AZ

RX(21) RCT B 84308-48-5, AR 17869-75-9
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO AZ 107345-28-8
 SOL 109-99-9 THF

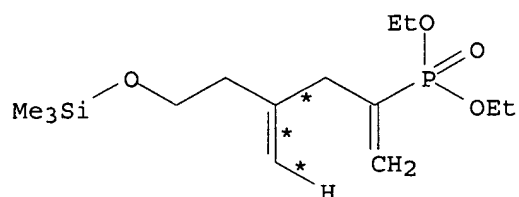
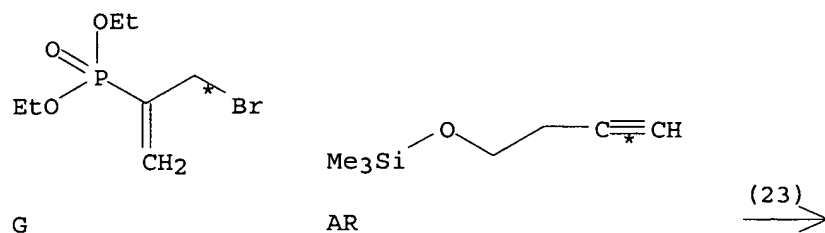
RX(22) OF 130 ...G + Z ==> BA...



BA

RX(22) RCT G 91476-10-7, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BA 107345-29-9
 SOL 109-99-9 THF

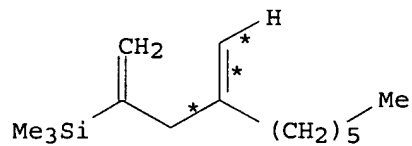
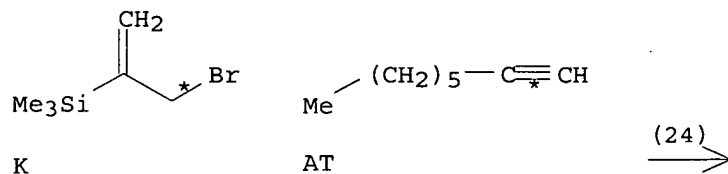
RX(23) OF 130 ...G + AR ==> BB...



BB

RX(23) RCT G 91476-10-7, AR 17869-75-9
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
 PRO BB 107345-30-2
 SOL 109-99-9 THF

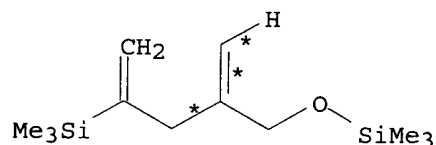
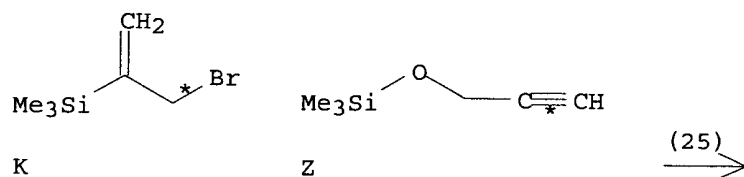
RX(24) OF 130 ...K + AT ==> BC



BC
YIELD 50%

RX(24) RCT K 91445-18-0, AT 629-05-0
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH2CH2Br
 PRO BC 94225-07-7
 SOL 109-99-9 THF

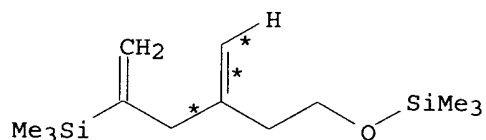
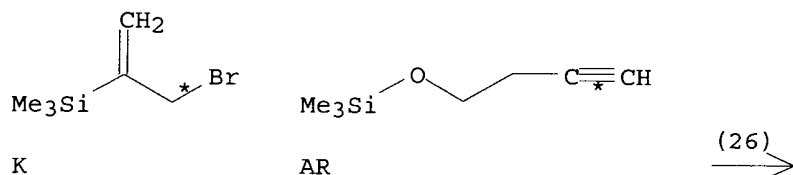
RX(25) OF 130 ...K + Z ==> BD



BD
YIELD 60%

RX(25) RCT K 91445-18-0, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BD 94225-08-8
 SOL 109-99-9 THF

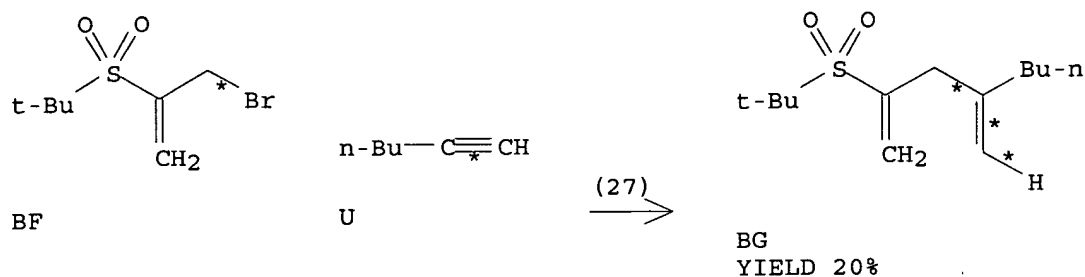
RX(26) OF 130 ...K + AR ==> BE



BE
YIELD 60%

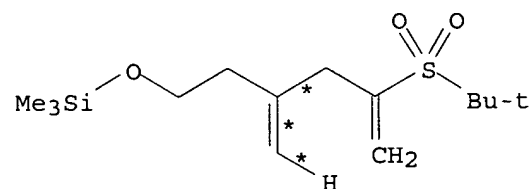
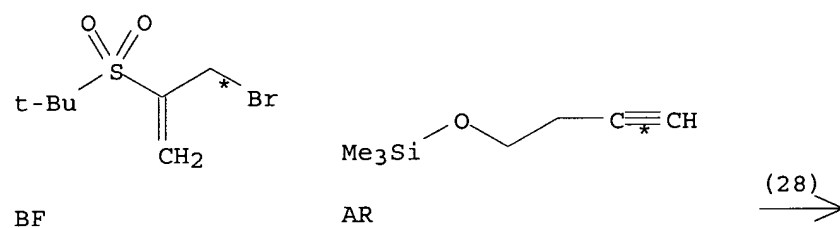
RX(26) RCT K 91445-18-0, AR 17869-75-9
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BE 94225-09-9
 SOL 109-99-9 THF

RX(27) OF 130 BF + U ==> BG



RX(27) RCT BF 97147-24-5, U 693-02-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BG 97779-27-6
 SOL 109-99-9 THF

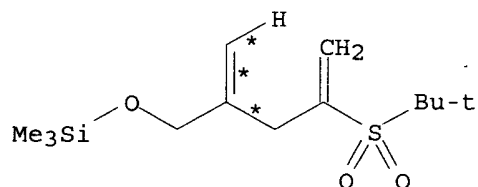
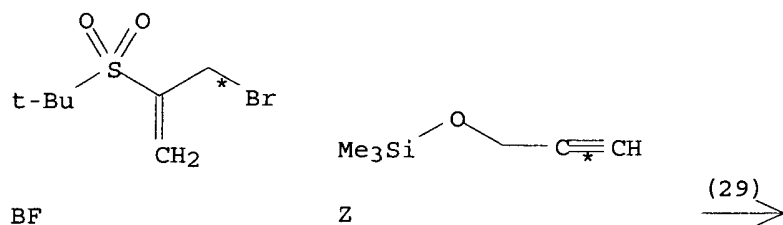
RX(28) OF 130 BF + AR ==> BH...



BH

RX(28) RCT BF 97147-24-5, AR 17869-75-9
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BH 107345-31-3
 SOL 109-99-9 THF

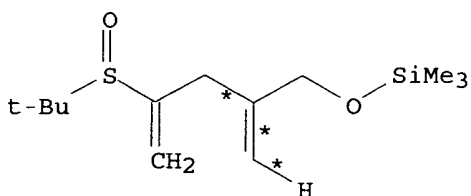
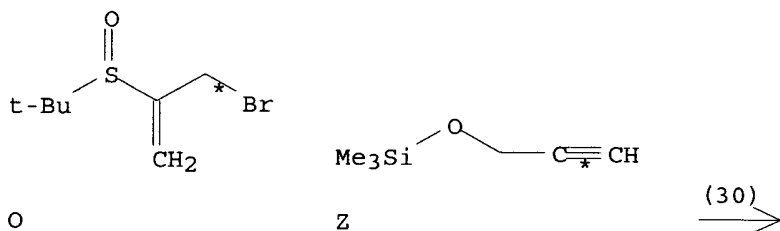
RX(29) OF 130 BF + Z ==> BI...



BI
YIELD 48%

RX(29) RCT BF 97147-24-5, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BI 107345-32-4
 SOL 109-99-9 THF

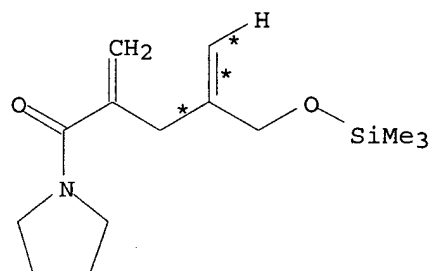
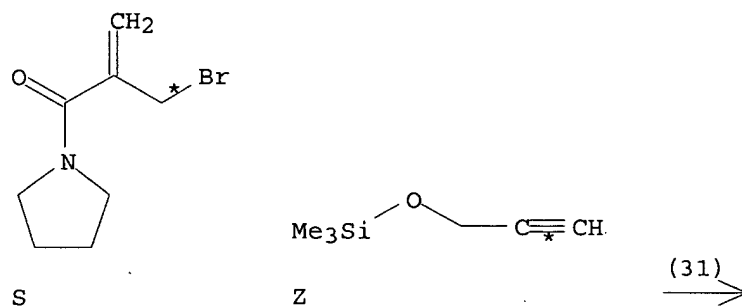
RX(30) OF 130 ...O + Z ==> BJ...



BJ

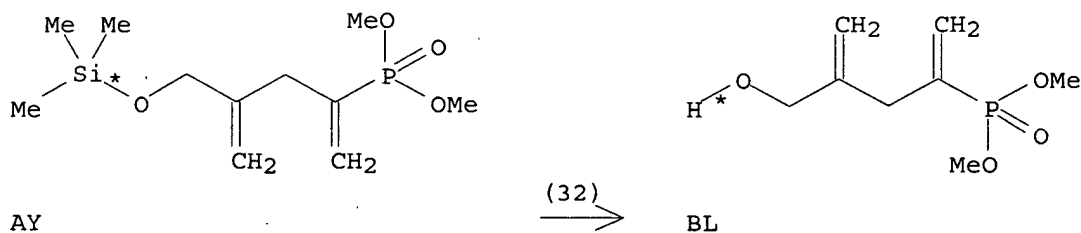
RX(30) RCT O 107345-23-3, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BJ 107345-33-5
 SOL 109-99-9 THF

RX(31) OF 130 ...S + Z ==> BK...



RX(31) RCT S 107345-24-4, Z 5582-62-7
 RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
 PRO BK 107345-34-6
 SOL 109-99-9 THF

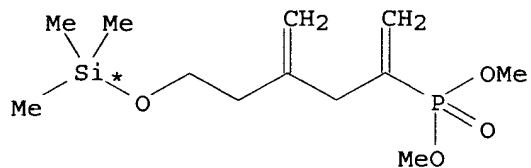
RX(32) OF 130 ...AY ==> BL...



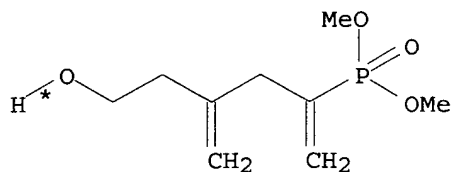
RX(32) RCT AY 107345-27-7
 RGT BM 7647-01-0 HCl
 PRO BL 91476-21-0
 SOL 7732-18-5 Water

RX(33) OF 130 ...AZ ==> BO...

3



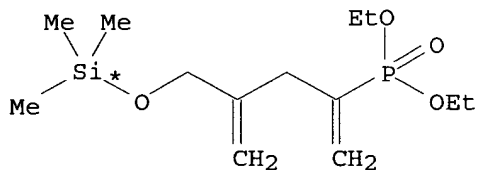
AZ



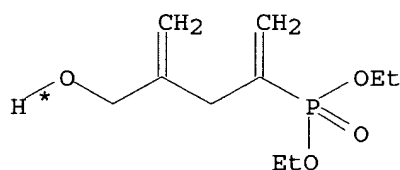
BO

RX(33) RCT AZ 107345-28-8
RGT BM 7647-01-0 HCl
PRO BO 91476-22-1
SOL 7732-18-5 Water

RX(34) OF 130 ...BA ==> BP...



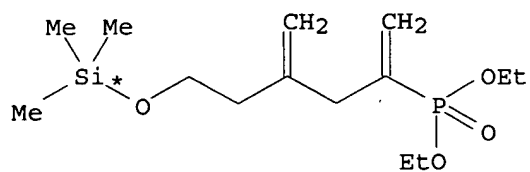
BA



BP

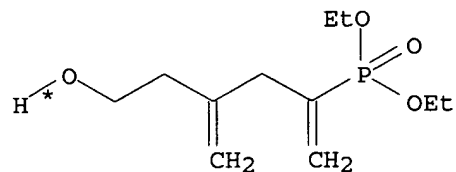
RX(34) RCT BA 107345-29-9
RGT BM 7647-01-0 HCl
PRO BP 91476-23-2
SOL 7732-18-5 Water

RX(35) OF 130 ...BB ==> BQ...



BB

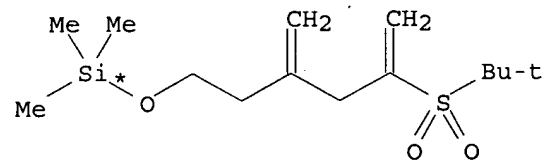
(35) →



BQ

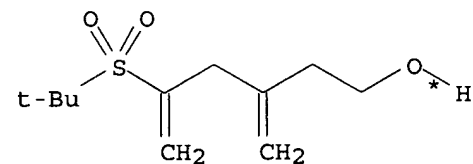
RX(35) RCT BB 107345-30-2
 RGT BM 7647-01-0 HCl
 PRO BQ 91476-24-3
 SOL 7732-18-5 Water

RX(36) OF 130 ...BH ==> BR



BH

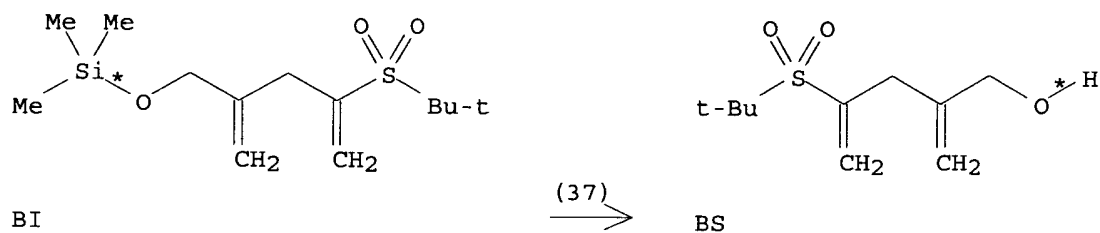
(36) →



BR

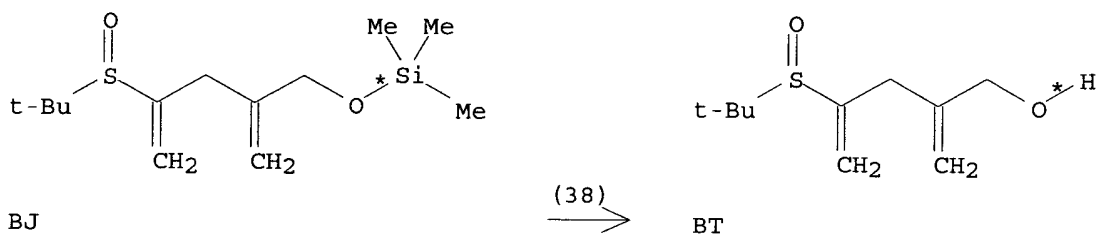
RX(36) RCT BH 107345-31-3
 RGT BM 7647-01-0 HCl
 PRO BR 97779-26-5
 SOL 7732-18-5 Water

RX(37) OF 130 ...BI ==> BS



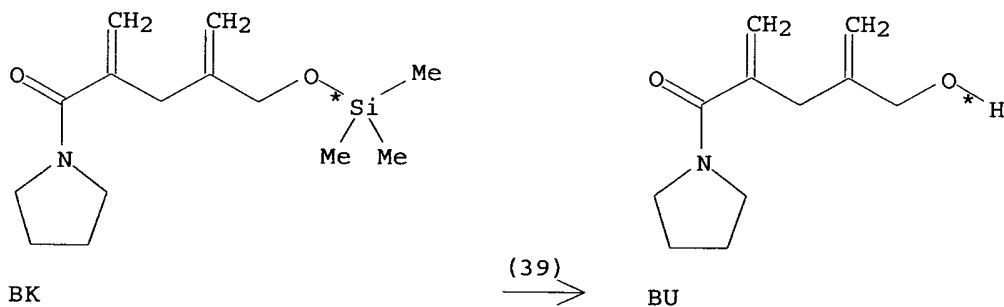
RX(37) RCT BI 107345-32-4
 RGT BM 7647-01-0 HCl
 PRO BS 97779-25-4
 SOL 7732-18-5 Water

RX(38) OF 130 ...BJ ==> BT



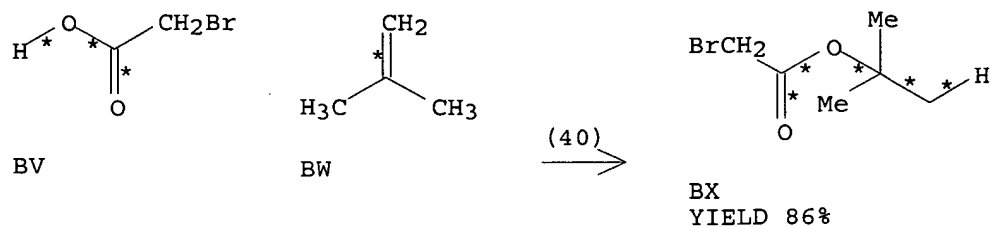
RX(38) RCT BJ 107345-33-5
 RGT BM 7647-01-0 HCl
 PRO BT 107345-35-7
 SOL 7732-18-5 Water

RX(39) OF 130 ...BK ==> BU



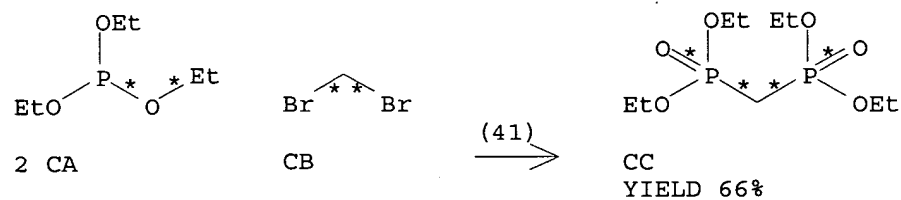
RX(39) RCT BK 107345-34-6
 RGT BM 7647-01-0 HCl
 PRO BU 107345-36-8
 SOL 7732-18-5 Water

RX(40) OF 130 BV + BW ==> BX



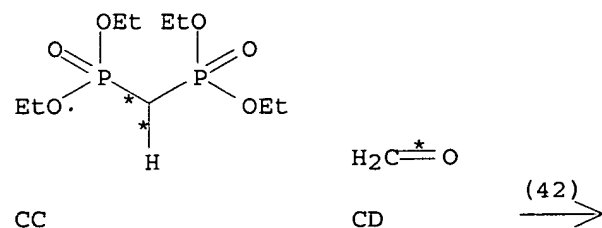
RX(40) RCT BV 79-08-3, BW 115-11-7
 RGT BY 9037-24-5 Amberlyst 15
 PRO BX 5292-43-3
 SOL 67-66-3 CHCl3

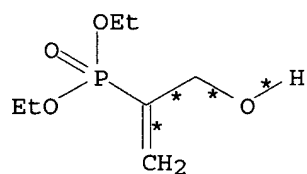
RX(41) OF 130 2 CA + CB ==> CC...



RX(41) RCT CA 122-52-1, CB 74-95-3
 PRO CC 1660-94-2

RX(42) OF 130 ...CC + CD ==> F...

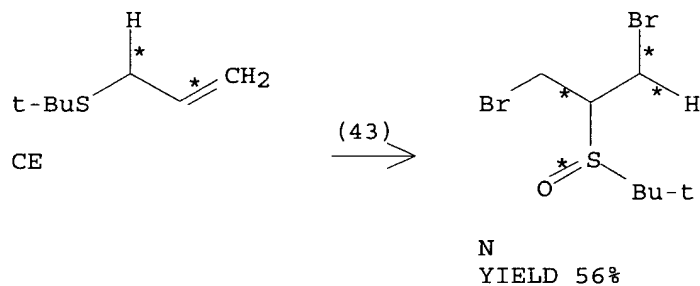




F
YIELD 60%

RX(42) RCT CC 1660-94-2, CD 50-00-0
PRO F 93032-43-0
SOL 7732-18-5 Water

RX(43) OF 130 CE ==> N...



RX(43) RCT CE 37850-75-2

STAGE(1)

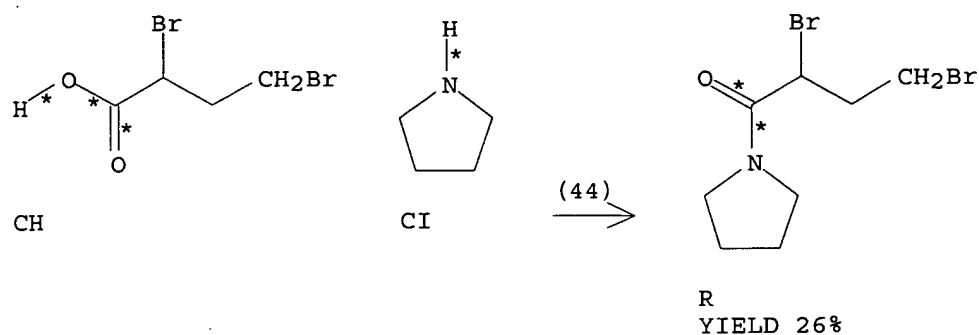
RGT CF 7726-95-6 Br2
SOL 56-23-5 CCl4

STAGE(2)

RGT CG 937-14-4 MCPBA
SOL 75-09-2 CH2Cl2

PRO N 107345-37-9

RX(44) OF 130 CH + CI ==> R...



RX(44) RCT CH 63164-16-9

STAGE(1)

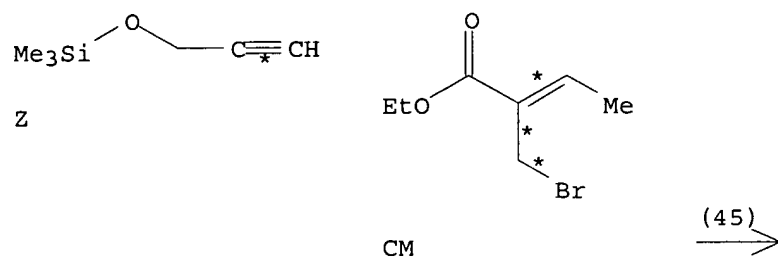
RGT CJ 7719-09-7 SOCl₂, CK 68-12-2 DMF
SOL 75-09-2 CH₂Cl₂

STAGE(2)

RCT CI 123-75-1
RGT CL 110-86-1 Pyridine
SOL 60-29-7 Et₂O

PRO R 107345-38-0

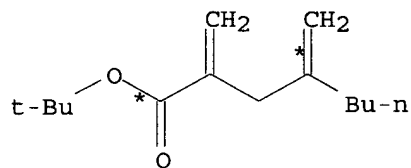
RX(45) OF 130 Z + CM ==> CN



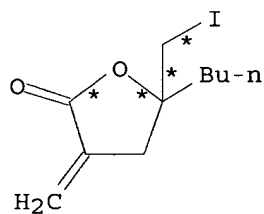
RX(45) RCT Z 5582-62-7, CM 62097-05-6
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br

PRO CN 107345-40-4
SOL 109-99-9 THF

RX(46) OF 130 ...V ==> CO



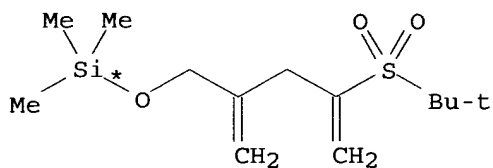
V



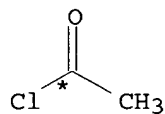
CO
YIELD 90%

RX(46) RCT V 91476-11-8
RGT CP 7553-56-2 I2, CQ 584-08-7 K2CO3
PRO CO 91476-25-4

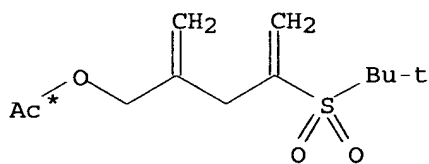
RX(47) OF 130 ...BI + AJ ==> CR...



BI



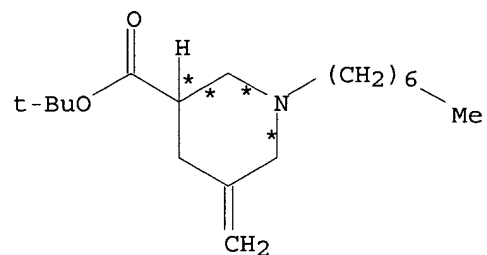
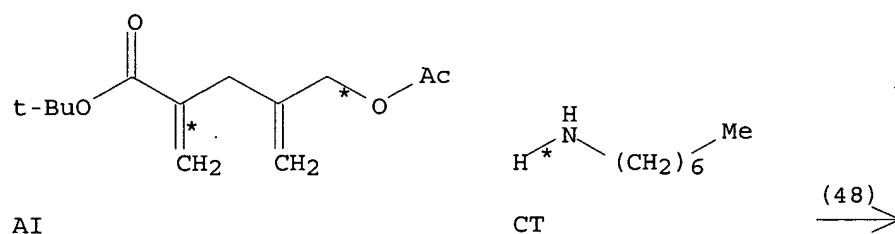
AJ



CR
YIELD 89%

RX(47) RCT BI 107345-32-4, AJ 75-36-5
 RGT AK 64-19-7 AcOH, CS 1122-58-3 4-DMAP
 PRO CR 107345-42-6
 SOL 60-29-7 Et2O, 64-19-7 AcOH

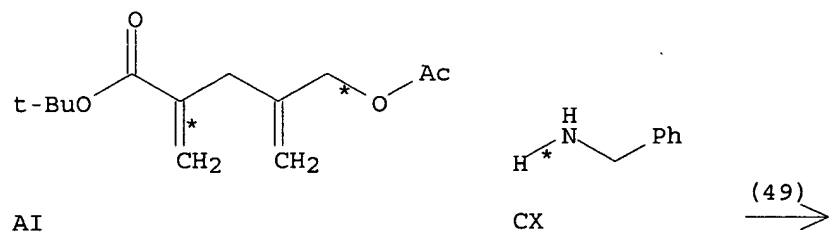
RX(48) OF 130 ...AI + CT ==> CU

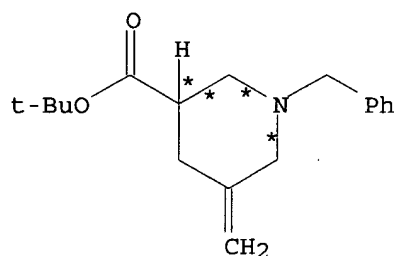


YIELD 82%

RX(48) RCT AI 91476-26-5, CT 111-68-2
 RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
 PRO CU 91476-28-7
 SOL 109-99-9 THF

RX(49) OF 130 ...AI + CX ==> CY

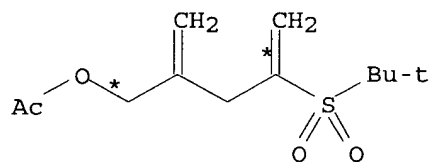




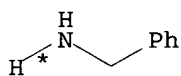
CY
YIELD 76%

RX(49) RCT AI 91476-26-5, CX 100-46-9
RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
PRO CY 91476-29-8
SOL 109-99-9 THF

RX(50) OF 130 ...CR + CX ==> CZ

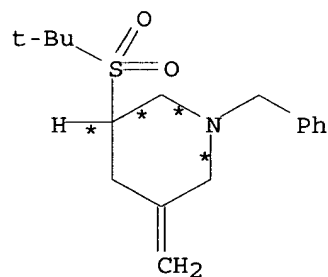


CR



CX

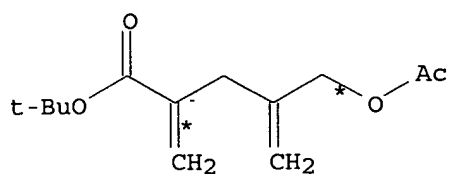
(50) →



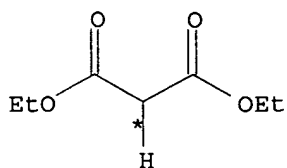
CZ
YIELD 90%

RX(50) RCT CR 107345-42-6, CX 100-46-9
RGT CW 14221-01-3 Pd(PPh3)4, DA 7646-69-7 NaH
PRO CZ 107345-43-7
SOL 109-99-9 THF

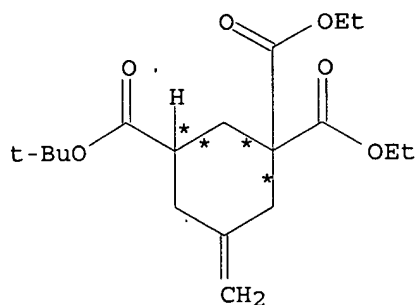
RX(51) OF 130 ...AI + DB ==> DC



AI



DB

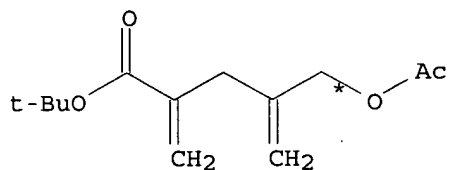
(51)
→

DC

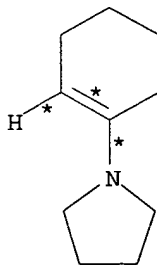
YIELD 70%

RX(51) RCT AI 91476-26-5, DB 105-53-3
 RGT CW 14221-01-3 Pd(PPh₃)₄, DA 7646-69-7 NaH
 PRO DC 91476-27-6
 SOL 109-99-9 THF

RX(52) OF 130 ...AI + DD ==> DE

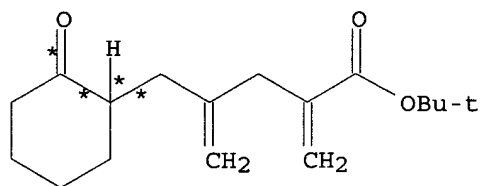


AI



DD

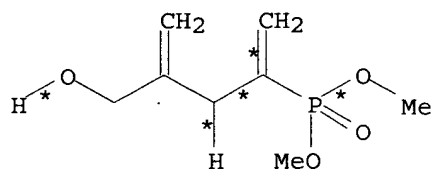
(52)
→



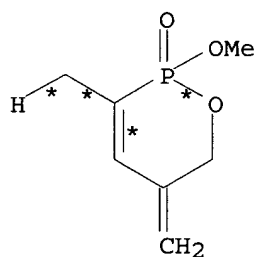
DE
YIELD 50%

RX(52) RCT AI 91476-26-5, DD 1125-99-1
RGT CV 121-44-8 Et3N, CW 14221-01-3 Pd(PPh3)4
PRO DE 91476-30-1
SOL 75-05-8 MeCN

RX(53) OF 130 ...BL ==> DG



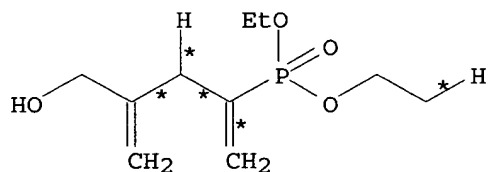
BL



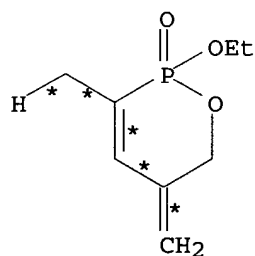
DG
YIELD 95%

RX(53) RCT BL 91476-21-0
RGT DA 7646-69-7 NaH
PRO DG 91476-31-2
SOL 109-99-9 THF

RX(54) OF 130 ...BP ==> DH



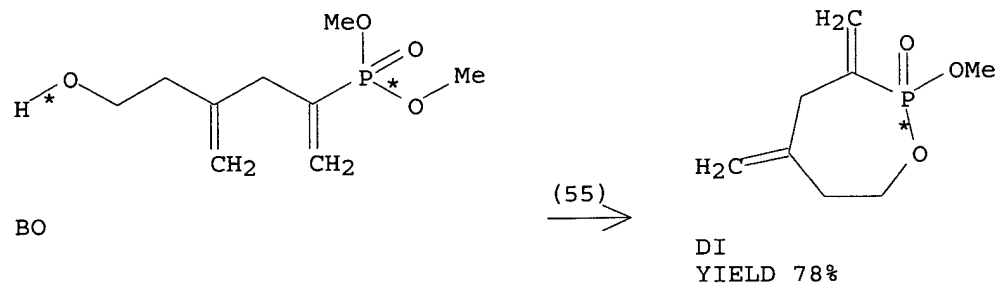
BP



DH
YIELD 95%

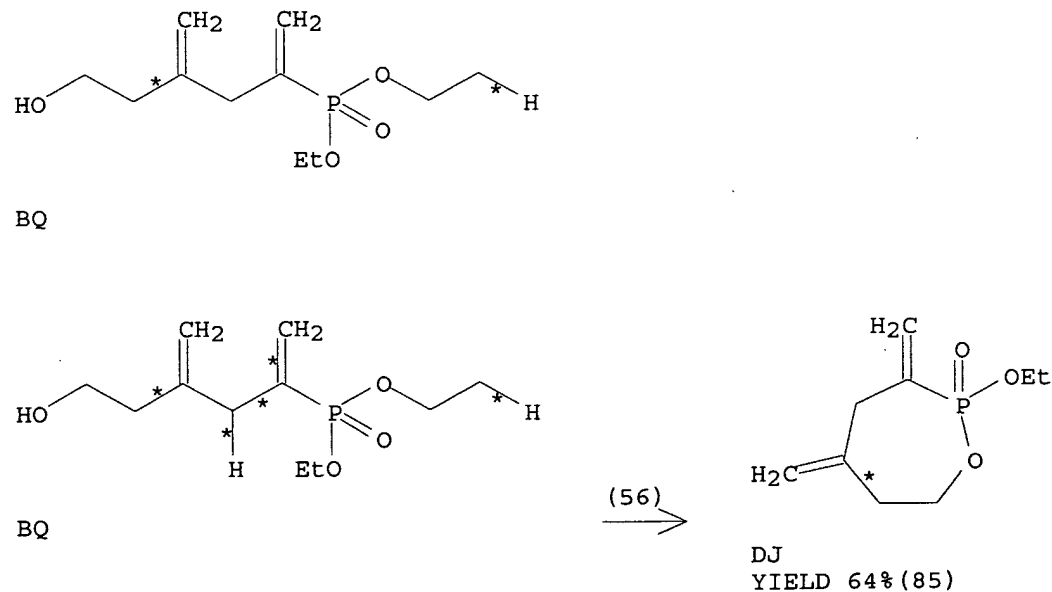
RX(54) RCT BP 91476-23-2
RGT DA 7646-69-7 NaH
PRO DH 91476-32-3
SOL 109-99-9 THF

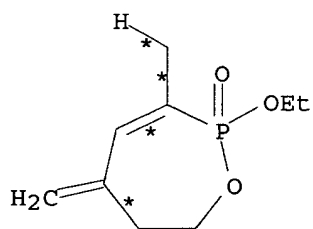
RX(55) OF 130 ...BO ==> DI



RX(55) RCT BO 91476-22-1
RGT DA 7646-69-7 NaH
PRO DI 91476-33-4
SOL 109-99-9 THF

RX(56) OF 130 ...2 BQ ==> DJ + DK

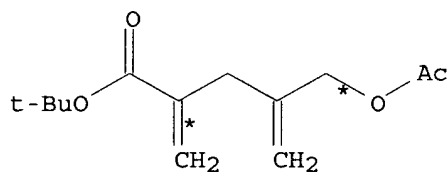




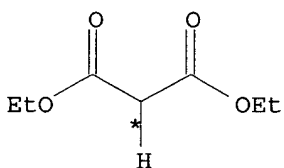
DK
YIELD 64% (15)

RX (56) RCT BQ 91476-24-3
 RGT DA 7646-69-7 NaH
 PRO DJ 107345-44-8, DK 107345-45-9
 SOL 109-99-9 THF

RX (51) OF 130 ...AI + DB ==> DC

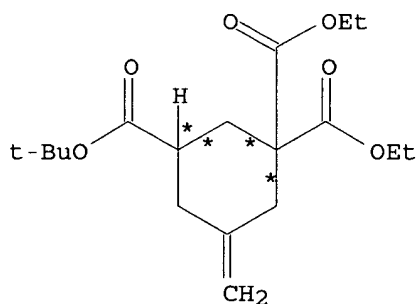


AI



DB

(51) \longrightarrow

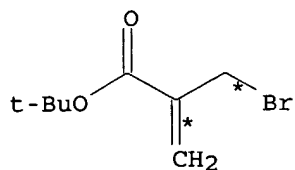


DC
YIELD 70%

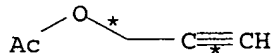
RX (51) RCT AI 91476-26-5, DB 105-53-3
 RGT CW 14221-01-3 Pd(PPh3)4, DA 7646-69-7 NaH
 PRO DC 91476-27-6
 SOL 109-99-9 THF

RX (71) OF 130 COMPOSED OF RX (11), RX (51)

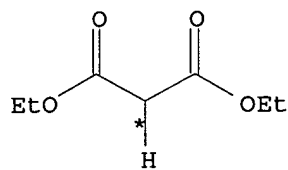
RX(71) T + AH + DB ==> DC



T

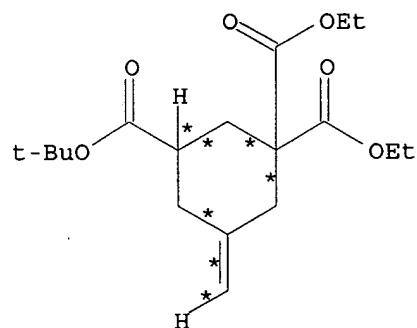


AH



DB

2
STEPS
→



DC

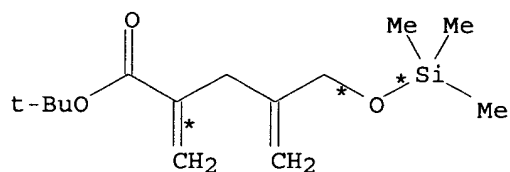
YIELD 70%

RX(11) RCT T 53913-96-5, AH 627-09-8
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AI 91476-26-5
SOL 109-99-9 THF

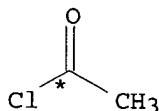
RX(51) RCT AI 91476-26-5, DB 105-53-3
RGT CW 14221-01-3 Pd(PPh₃)₄, DA 7646-69-7 NaH
PRO DC 91476-27-6
SOL 109-99-9 THF

RX(75) OF 130 COMPOSED OF RX(12), RX(51)

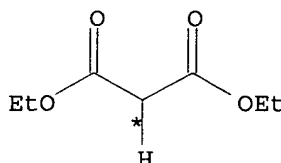
RX(75) AA + AJ + DB ==> DC



AA

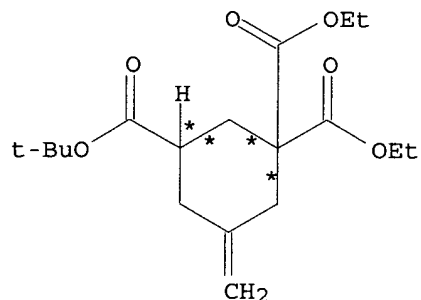


AJ



DB

2
STEPS
→



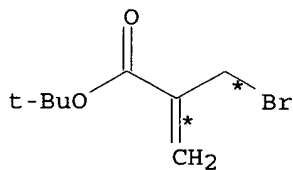
DC
YIELD 70%

RX(12) RCT AA 91476-12-9, AJ 75-36-5
RGT AK 64-19-7 AcOH
PRO AI 91476-26-5
SOL 60-29-7 Et2O, 64-19-7 AcOH

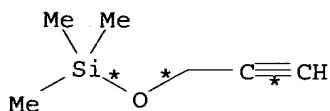
RX(51) RCT AI 91476-26-5, DB 105-53-3
RGT CW 14221-01-3 Pd(PPh3)4, DA 7646-69-7 NaH
PRO DC 91476-27-6
SOL 109-99-9 THF

RX(107) OF 130 COMPOSED OF RX(7), RX(12), RX(51)

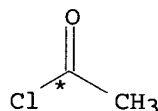
RX(107) T + Z + AJ + DB ==> DC



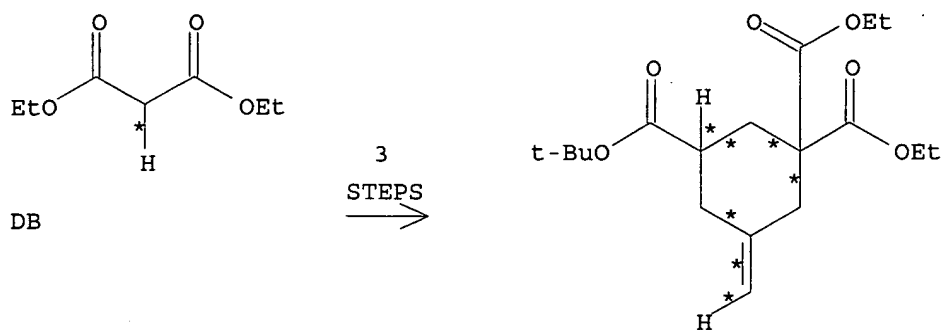
T



Z



AJ



DC
YIELD 70%

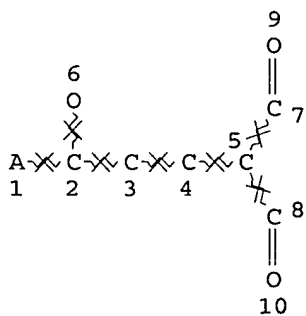
RX(7) RCT T 53913-96-5, Z 5582-62-7
RGT W 7440-66-6 Zn, X 106-93-4 BrCH₂CH₂Br
PRO AA 91476-12-9
SOL 109-99-9 THF

RX(12) RCT AA 91476-12-9, AJ 75-36-5
RGT AK 64-19-7 AcOH
PRO AI 91476-26-5
SOL 60-29-7 Et₂O, 64-19-7 AcOH

RX(51) RCT AI 91476-26-5, DB 105-53-3
RGT CW 14221-01-3 Pd(PPh₃)₄, DA 7646-69-7 NaH
PRO DC 91476-27-6
SOL 109-99-9 THF

=> => d que stat 193

L21 SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010
L25 STR



NODE ATTRIBUTES:

CONNECT IS X2 RC AT 6
CONNECT IS E1 RC AT 9
CONNECT IS E1 RC AT 10
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

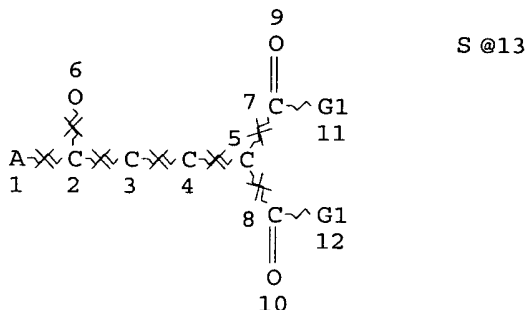
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L27 12118 SEA FILE=REGISTRY SSS FUL L25 NOT L21

L30 STR



VAR G1=O/N/P/13

NODE ATTRIBUTES:

CONNECT IS X2 RC AT 6

CONNECT IS E1 RC AT 9

CONNECT IS E1 RC AT 10

CONNECT IS X2 RC AT 13

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

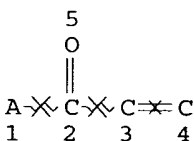
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L32 2503 SEA FILE=REGISTRY SUB=L27 SSS FUL L30

L37 STR



NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L40 SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005

L42 6815 SEA FILE=REGISTRY SSS FUL L37 NOT L40

L50 1507 SEA FILE=HCAPLUS ABB=ON PLU=ON L32/P

L51 31232 SEA FILE=HCAPLUS ABB=ON PLU=ON L42/RACT

L52 266 SEA FILE=HCAPLUS ABB=ON PLU=ON L50 AND L51

L53 QUE ABB=ON PLU=ON "ASYMMETRIC SYNTHESIS AND INDUCTION"+PFT,OLD,NT/CT

L54 QUE ABB=ON PLU=ON "MICHAEL REACTION"+PFT,OLD,NT/CT

L55 QUE ABB=ON PLU=ON "MICHAEL REACTION CATALYSTS"+PFT,O

LD,NT/CT

L56 30 SEA FILE=HCAPLUS ABB=ON PLU=ON L53 AND L52
L57 21 SEA FILE=HCAPLUS ABB=ON PLU=ON L56 AND (L54 OR L55)
L60 31232 SEA FILE=HCAPLUS ABB=ON PLU=ON L42/RACT
L61 1337 SEA FILE=HCAPLUS ABB=ON PLU=ON L60 AND L53
L62 176 SEA FILE=HCAPLUS ABB=ON PLU=ON L61 AND (L54 OR L55)
L63 92 SEA FILE=HCAPLUS ABB=ON PLU=ON L62 AND L55
L64 744935 SEA FILE=REGISTRY ABB=ON PLU=ON ((FE OR CO OR NI OR
RU OR RH OR PD OR OS OR IR OR PT) (L)N)/ELS
L66 316118 SEA FILE=REGISTRY ABB=ON PLU=ON L64 AND 1-2/N
L67 262888 SEA FILE=REGISTRY ABB=ON PLU=ON L66 AND 1/M
L68 22790 SEA FILE=REGISTRY ABB=ON PLU=ON L67 AND 1/RU
L69 80253 SEA FILE=REGISTRY ABB=ON PLU=ON L67 AND (1/OS OR
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L82 31 SEA FILE=HCAPLUS ABB=ON PLU=ON L80 AND L81 AND L77
L83 7 SEA FILE=HCAPLUS ABB=ON PLU=ON L82 AND L53
L84 1971 SEA FILE=HCAPLUS ABB=ON PLU=ON L32
L85 315 SEA FILE=HCAPLUS ABB=ON PLU=ON L84 AND L42
L86 14 SEA FILE=HCAPLUS ABB=ON PLU=ON L85 AND L77
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L86
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OR L55)
L92 QUE ABB=ON PLU=ON PY<2005 OR PRY<2005 OR AY<2005 OR
MY<2005 OR REVIEW/DT
L93 34 SEA FILE=HCAPLUS ABB=ON PLU=ON L90 AND L92

=> d l93 1-34 ibib abs ed hitstr hitind

L93 ANSWER 1 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:792305 HCAPLUS

DOCUMENT NUMBER: 141:424327

TITLE: Enantioselective total synthesis of
(-)-strychnine: development of a highly
practical catalytic asymmetric carbon-carbon
bond formation and domino cyclization

AUTHOR(S): Ohshima, Takashi; Xu, Youjun; Takita, Ryo;
Shibasaka, Masakatsu

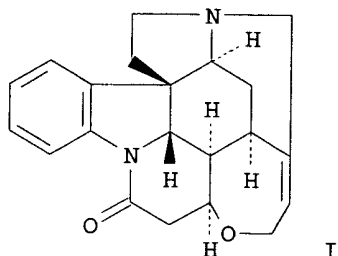
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Hongo, Bunkyo-ku,
Tokyo, 113-0033, Japan

SOURCE: Tetrahedron (2004), 60(43),
9569-9588

CODEN: TETRAB; ISSN: 0040-4020

PUBLISHER: Elsevier B.V.

DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:424327
 GI



AB An enantioselective total synthesis of (-)-strychnine (I) was accomplished through the use of the highly practical catalytic asym. Michael reaction (0.1 mol% of (R)-ALB, greater than kilogram scale, without chromatog., 91% yield and >99% ee), and a domino cyclization that simultaneously constructed the B- and D- rings of strychnine (>77% yield). Newly-developed reaction conditions for thionium ion cyclization, NaBH₃CN reduction of the imine moiety in the presence of a Lewis acid to prevent the ring-opening reaction, and chemoselective reduction of the thioether (desulfurization) in the presence of exocyclic olefin were pivotal to complete the synthesis. The described chemical paves the way for the synthesis of more advanced Strychnos alkaloids.

ED Entered STN: 29 Sep 2004

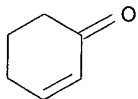
IT 930-68-7, 2-Cyclohexenone

RL: RCT (Reactant); RACT (Reactant or reagent)

(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 164931-77-5P

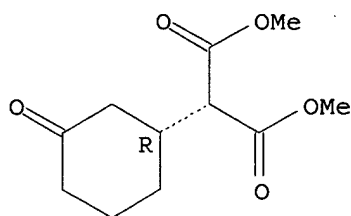
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 31-5 (Alkaloids)

IT **Asymmetric synthesis and induction**

Cyclization

(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

IT **Michael reaction**

(stereoselective; enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

IT 108-59-8, Dimethyl malonate 126-39-6 609-73-4,
 1-Iodo-2-nitrobenzene 661-69-8, Hexamethyldistannane
 930-68-7, 2-Cyclohexenone 22483-09-6 122807-21-0
 191731-32-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

IT 509-40-0P, Diaboline 71366-23-9P 76074-18-5P
 164931-77-5P 482351-05-3P 482351-06-4P 482351-07-5P
 482351-08-6P 482351-09-7P 482351-10-0P 482351-11-1P
 482351-12-2P 482351-13-3P 482351-14-4P 482351-15-5P
 482351-16-6P 482351-18-8P 482351-19-9P 482351-20-2P
 482351-22-4P 482351-24-6P 482351-25-7P 482351-26-8P
 482351-27-9P 482351-28-0P 482351-29-1P 482351-31-5P
 793723-96-3P 793723-97-4P 793723-98-5P 793724-03-5P
 793724-04-6P 793724-09-1P 793724-10-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(enantioselective total synthesis of (-)-strychnine via catalytic asym. Michael reaction and domino cyclization)

REFERENCE COUNT: 103 THERE ARE 103 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

193 ANSWER 2 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:584477 HCAPLUS

DOCUMENT NUMBER: 141:140101

TITLE: Process and catalysts for producing optically active cycloalkylmalonates

INVENTOR(S): Watanabe, Masahito; Murata, Kunihiro; Ikariya, Takao

PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki Kaisha, Japan

SOURCE: Eur. Pat. Appl., 29 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.

KIND

DATE

APPLICATION NO.

DATE

EP 1439159 A1 20040721 EP 2004-296

2004
0109

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ,
EE, HU, SK

JP 2004269481 A2 20040930 JP 2003-71368

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US 2004176616	A1	20040909	US 2003-749806	2003
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PRIORITY APPLN. INFO.:

JP 2003-9786 A

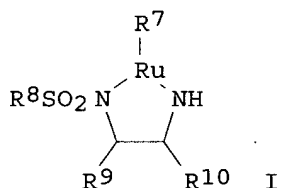
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JP 2003-71368      A
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                    0317

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OTHER SOURCE(S) : MARPAT 141:140101
GI



AB Optically active malonate derivs. R1COCR2R3CR4(COXR5)COYR6 [R1 = (un)substituted aromatic, aliphatic, alicyclic, heterocyclic, H, alkoxy, amino; R2-R4 = H, (un)substituted aryl, aliphatic, alicyclic, heterocyclic; R1R2, R1R3, R2R3, R4R5, R5R6, R4R6 = atoms required to form a ring; R5, R6 = H, (un)substituted aryl, aliphatic, alicyclic, alkoxy; X, Y = bond; XR5, YR6 = (un)substituted OH, NH2] were prepared by treating R1COCH:CR2R3 with R4CH(COXR5)COYR6 in presence of an asym. metal catalyst, preferably a Ru catalyst I [R7-R10 = (un)substituted Ph]. Thus, [RuCl2(C6Me6)]2 was treated with (S,S)-TsDPEN to give Ru[(S,S)-TsDPEN](C6Me6) which was used in the Michael reaction of 2-cyclohexenone with CH2(CO2Me)2 to give (R)-3-[bis(methoxycarbonyl)methyl]cyclohexanone in 96% ee.

ED Entered STN: 22 Jul 2004

IT 725737-68-8P

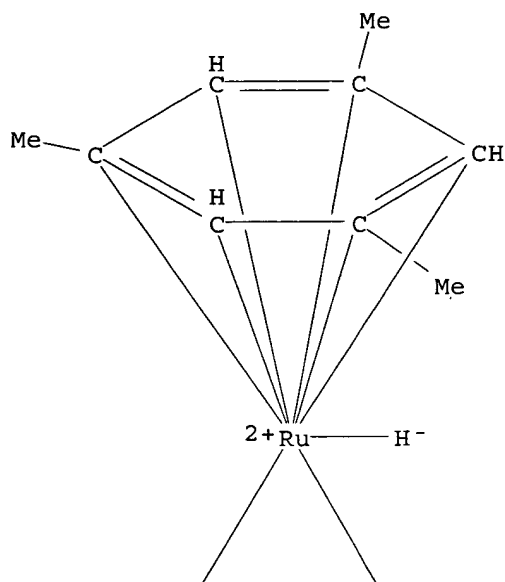
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(process and catalysts for producing optically active cycloalkylmalonates)

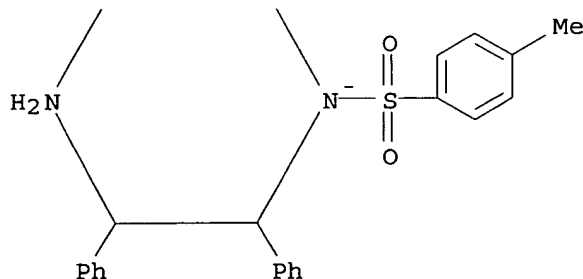
RN 725737-68-8 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato-κN]hydro[(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



IT 188444-42-0P 725737-67-7P 725737-69-9P

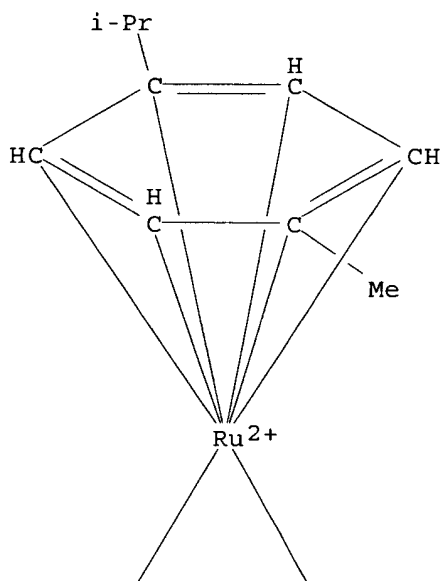
725737-70-2P 725737-71-3P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)

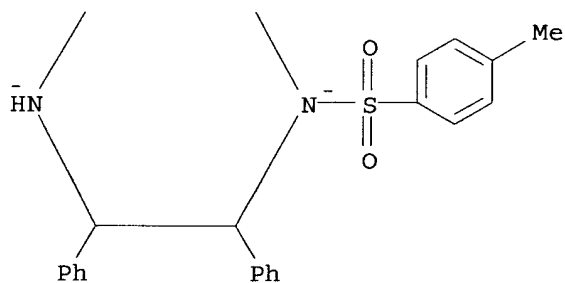
RN 188444-42-0 HCAPLUS

CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

PAGE 1-A

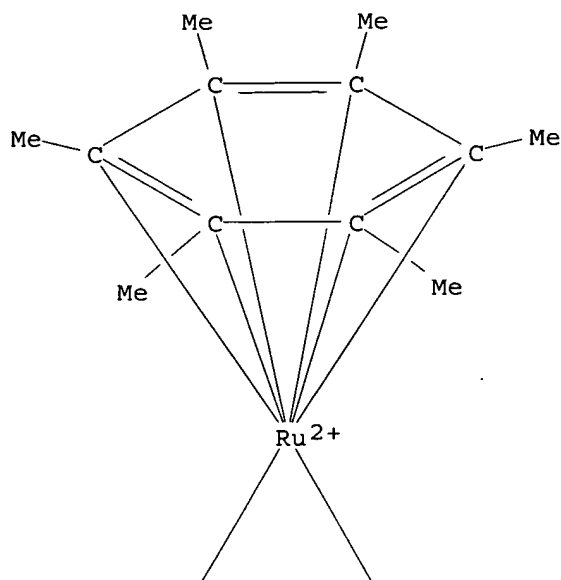


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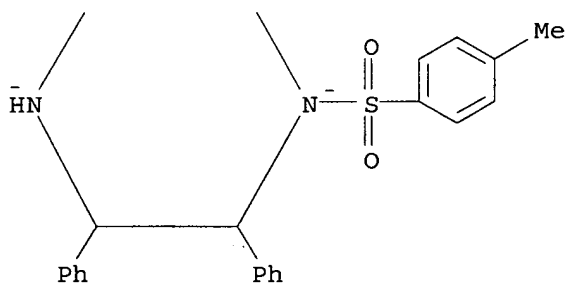


RN 725737-67-7 HCAPLUS
 CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

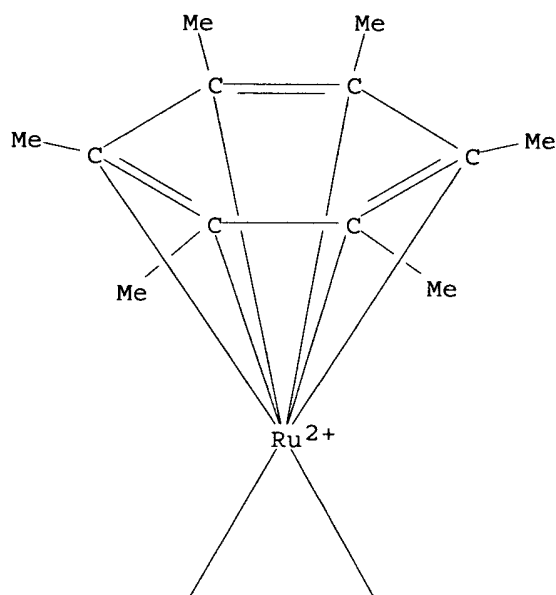


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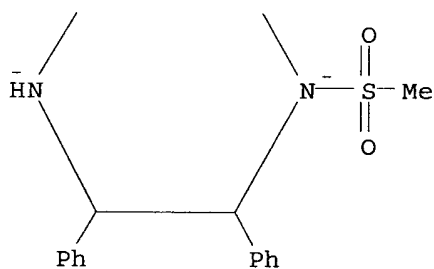


RN 725737-69-9 HCAPLUS
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PAGE 1-A

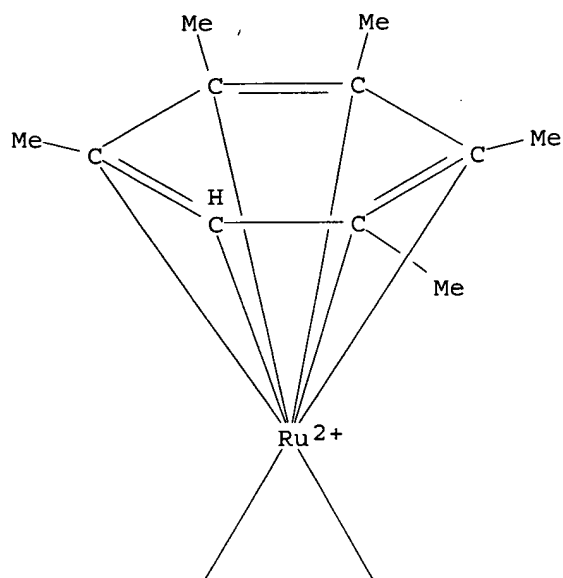


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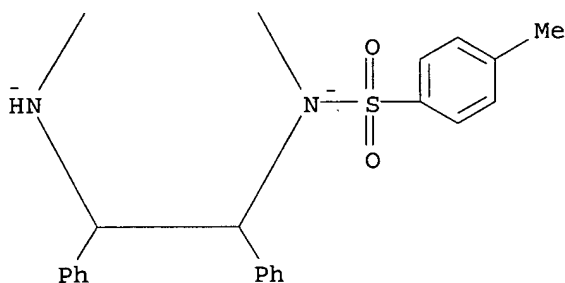


RN 725737-70-2 HCAPLUS
 CN Ruthenium, [N-[(1S,2S)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-pentamethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A



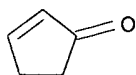
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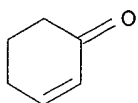
RN 725737-71-3 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN](dimethylpropanedioate-κO1',κO3')[(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]-(9CI) (CA INDEX NAME)

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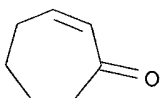
IT 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexenone 1121-66-0; 2-Cycloheptenone
 22748-16-9, 4,4-Dimethyl-2-cyclopentenone
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (process and catalysts for producing optically active
 cycloalkylmalonates)
 RN 930-30-3 HCAPLUS
 CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



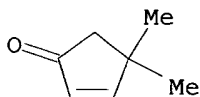
RN 930-68-7 HCAPLUS
 CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS
 CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

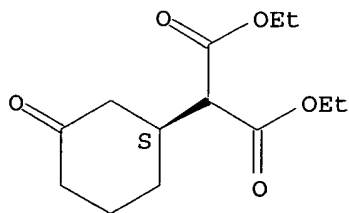


RN 22748-16-9 HCAPLUS
 CN 2-Cyclopenten-1-one, 4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 151600-50-9P 287493-82-7P 724774-83-8P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (process and catalysts for producing optically active cycloalkylmalonates)
 RN 151600-50-9 HCAPLUS
 CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI)
 (CA INDEX NAME)

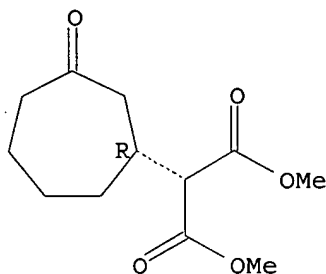
Absolute stereochemistry. Rotation (-).



RN 287493-82-7 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)

(CA INDEX NAME)

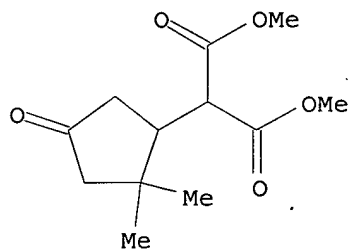
Absolute stereochemistry. Rotation (+).



RN 724774-83-8 HCAPLUS

CN Propanedioic acid, (2,2-dimethyl-4-oxocyclopentyl)-, dimethyl ester, (+)- (9CI) (CA INDEX NAME)

Rotation (+).



IT 154194-50-0P 160115-23-1P 164931-77-5P

164931-78-6P 173837-41-7P 193530-87-9P

194095-90-4P 287493-81-6P 568590-07-8P

569342-29-6P 724774-82-7P, 3-[1,1-

Bis(methoxycarbonyl)ethyl]cyclopentanone 724774-84-9P,

3-[(Acetyl)(methoxycarbonyl)methyl]cyclopentanone

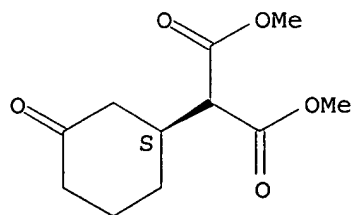
RL: SPN (Synthetic preparation); PREP (Preparation)

(process and catalysts for producing optically active cycloalkylmalonates)

RN 154194-50-0 HCAPLUS

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(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

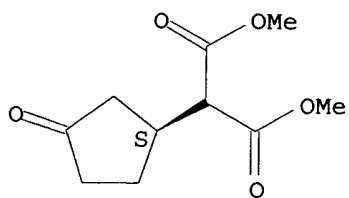


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(CA INDEX NAME)

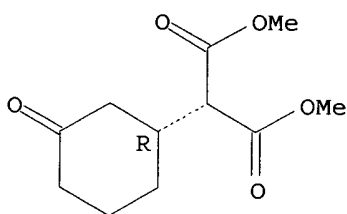
Absolute stereochemistry. Rotation (-).



RN 164931-77-5 HCAPLUS

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(CA INDEX NAME)

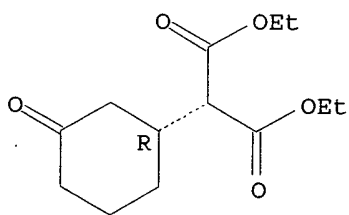
Absolute stereochemistry. Rotation (+).



RN 164931-78-6 HCAPLUS

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(CA INDEX NAME)

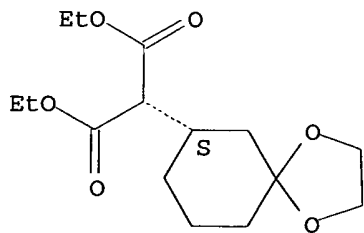
Absolute stereochemistry. Rotation (+).



RN 173837-41-7 HCAPLUS

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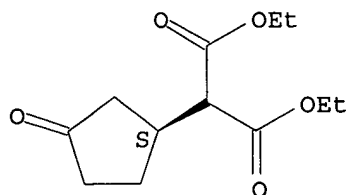
Absolute stereochemistry.



RN 193530-87-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

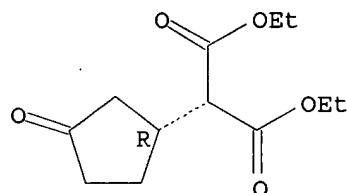
Absolute stereochemistry. Rotation (-).



RN 194095-90-4 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

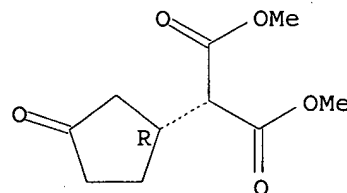
Absolute stereochemistry. Rotation (+).



RN 287493-81-6 HCAPLUS

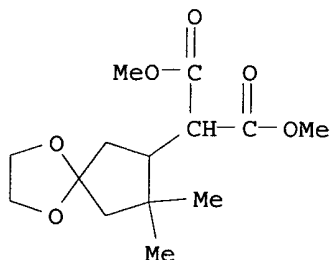
CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 568590-07-8 HCAPLUS

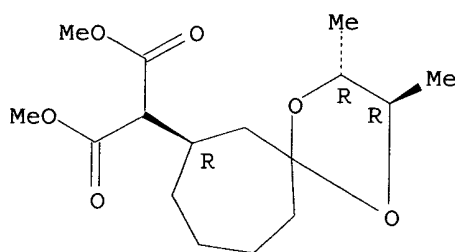
CN Propanedioic acid, (8,8-dimethyl-1,4-dioxaspiro[4.4]non-7-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 569342-29-6 HCAPLUS

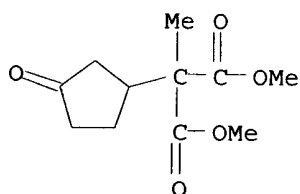
CN Propanedioic acid, [(2R,3R,7R)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



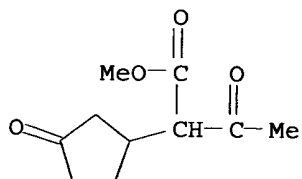
RN 724774-82-7 HCAPLUS

CN Propanedioic acid, methyl(3-oxocyclopentyl)-, dimethyl ester (9CI)
(CA INDEX NAME)



RN 724774-84-9 HCAPLUS

CN Cyclopentaneacetic acid, alpha-acetyl-3-oxo-, methyl ester (9CI)
(CA INDEX NAME)



IC ICM C07C045-72

CC 24-5 (Alicyclic Compounds)

- IT **Asymmetric synthesis and induction**
(process and catalysts for producing optically active cycloalkylmalonates)
- IT **Michael reaction**
Michael reaction catalysts
(stereoselective; process and catalysts for producing optically active cycloalkylmalonates)
- IT **725737-68-8P**
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)
- IT **188444-42-0P 725737-67-7P 725737-69-9P 725737-70-2P 725737-71-3P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(process and catalysts for producing optically active cycloalkylmalonates)
- IT 105-45-3, Methyl acetoacetate 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate 126-39-6, 2-Butanone ethyleneketal 609-02-9, Dimethyl methylmalonate 930-30-3, 2-Cyclopentenone 930-68-7, 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone 22748-16-9, 4,4-Dimethyl-2-cyclopentenone 24347-58-8, (2R,3R)-2,3-Butanediol 67421-02-7 167316-27-0
RL: RCT (Reactant); RACT (Reactant or reagent)
(process and catalysts for producing optically active cycloalkylmalonates)
- IT **151600-50-9P 287493-82-7P 724774-83-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(process and catalysts for producing optically active cycloalkylmalonates)
- IT **154194-50-0P 160115-23-1P 164931-77-5P 164931-78-6P 173837-41-7P 193530-87-9P 194095-90-4P 287493-81-6P 568590-07-8P 569342-29-6P 724774-82-7P, 3-[1,1-Bis(methoxycarbonyl)ethyl]cyclopentanone 724774-84-9P, 3-[(Acetyl)(methoxycarbonyl)methyl]cyclopentanone**
RL: SPN (Synthetic preparation); PREP (Preparation)
(process and catalysts for producing optically active cycloalkylmalonates)

L93 ANSWER 3 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:278187 HCAPLUS

DOCUMENT NUMBER: 141:71293

TITLE: Asymmetric Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes

AUTHOR(S): Ikariya, Takao; Wang, Hui; Watanabe, Masahito; Murata, Kunihiro

CORPORATE SOURCE: Graduate School of Science and Engineering, Department of Applied Chemistry, Tokyo Institute of Technology and Frontier Collaborative Research Center, Meguro-ku, Tokyo, 152-8552, Japan

SOURCE: Journal of Organometallic Chemistry (2004), 689(8), 1377-1381

PUBLISHER: CODEN: JORCAI; ISSN: 0022-328X
 Elsevier Science B.V.
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 141:71293

AB Well-defined 16-electron chiral Ru amido complexes, Ru[(R,R)-diamine](η^6 -arene), efficiently catalyze asym. Michael addns. of Michael donors to cyclic enones to give adducts in high yields and with excellent ee's. β -Keto esters or nitroacetate as Michael donors react with 2-cyclopentenone in toluene or Me₃COH containing the Ru amido catalyst (S/C = 50) to afford the Michael adduct in 99% yield and with up to 92% ee. The outcome of the reaction was delicately influenced by the structures of the diamine and arene ligands as well as reaction conditions.

ED Entered STN: 05 Apr 2004

IT 195516-84-8 569336-64-7 569336-66-9

618912-25-7 709674-02-2 709674-03-3

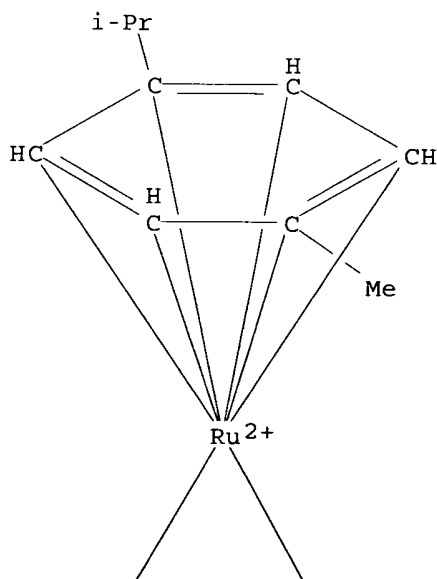
RL: CAT (Catalyst use); USES (Uses)

(asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

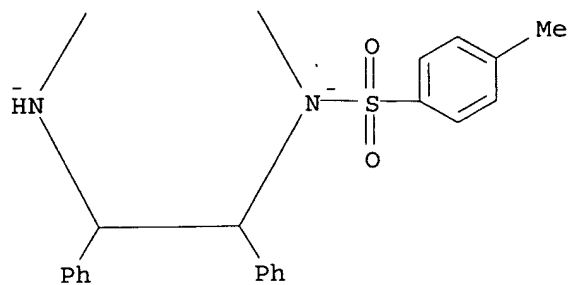
RN 195516-84-8 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)- κ N][(1,2,3,4,5,6- η)-1-methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

PAGE 1-A

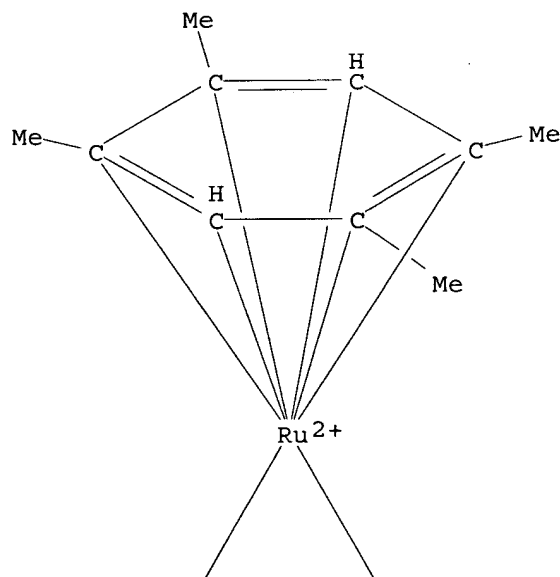


PAGE 2-A

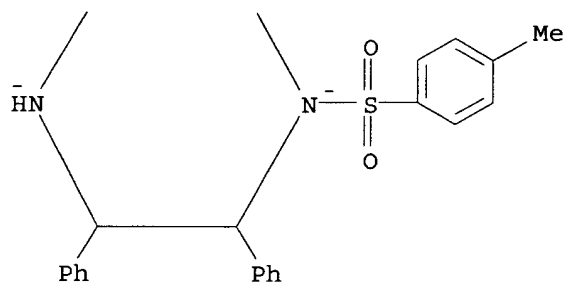


RN 569336-64-7 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-1,2,4,5-tetramethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

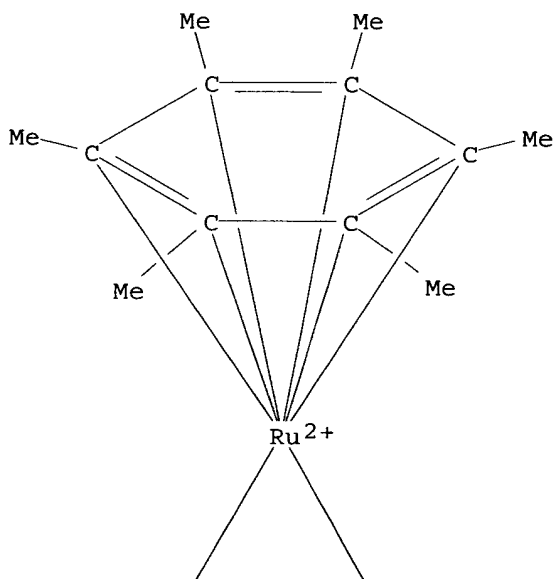


PAGE 2-A

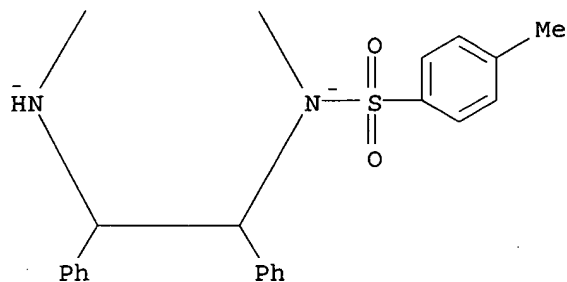


RN 569336-66-9 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

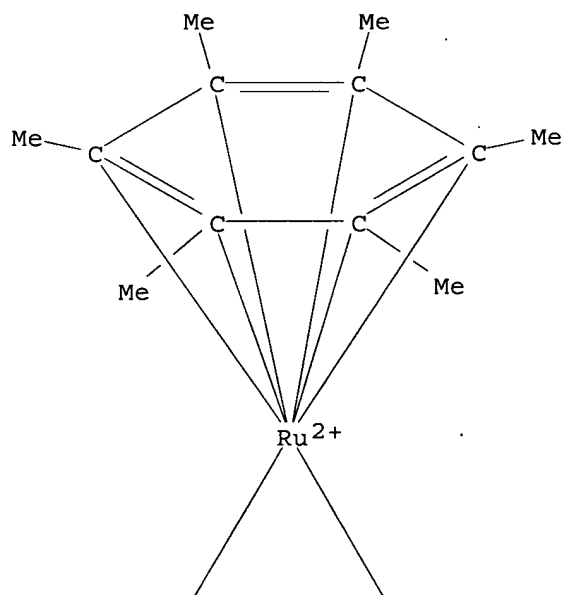


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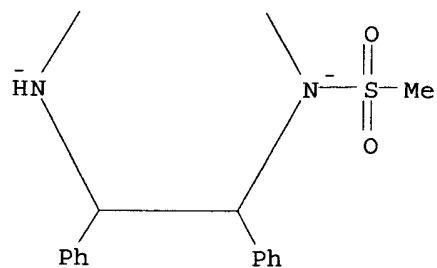


RN 618912-25-7 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]methanesulfonamid
ato(2-)-κN] [(1,2,3,4,5,6-η)-hexamethylbenzene] - (9CI)
(CA INDEX NAME)

PAGE 1-A

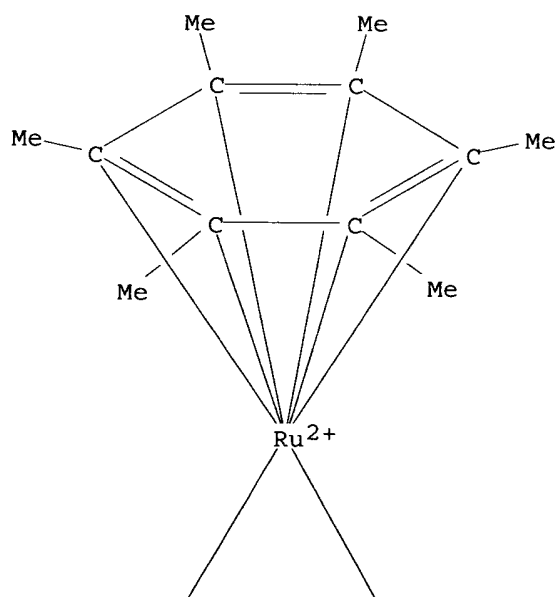


PAGE 2-A

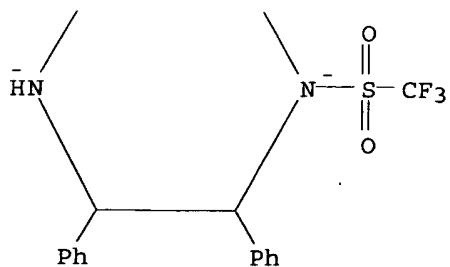


RN 709674-02-2 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-1,1,1-trifluoromethanesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

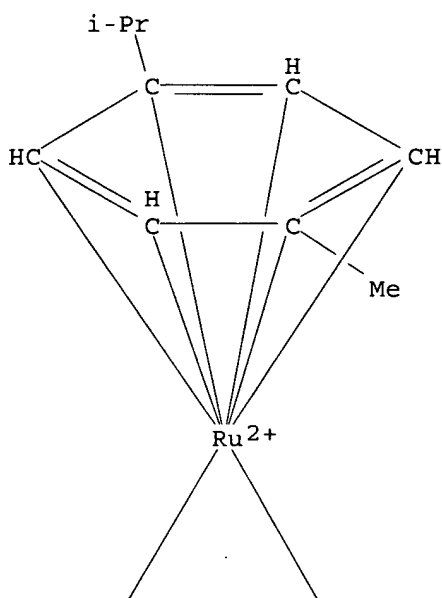


PAGE 2-A

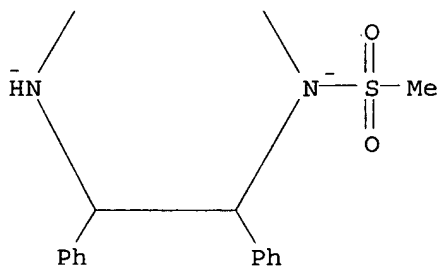


RN 709674-03-3 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino- κ N)-1,2-diphenylethyl]methanesulfonamidato(2-)- κ N] [(1,2,3,4,5,6- η)-1-methyl-4-(1-methylethyl)benzene] - (9CI) (CA INDEX NAME)

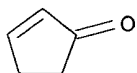
PAGE 1-A



PAGE 2-A



IT 930-30-3, 2-Cyclopenten-1-one
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. Michael reactions of α -substituted acetates with
 cyclic enones catalyzed by multifunctional chiral Ru amido
 complexes)
 RN 930-30-3 HCAPLUS
 CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



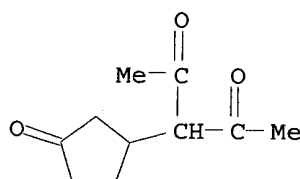
IT 94410-50-1P 160115-23-1P 646038-06-4P

708266-26-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reactions of α -substituted acetates with
cyclic enones catalyzed by multifunctional chiral Ru amido
complexes)

RN 94410-50-1 HCAPLUS

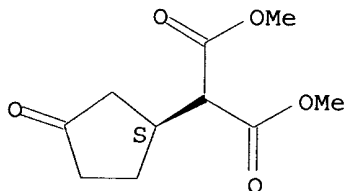
CN 2,4-Pentanedione, 3-(3-oxocyclopentyl)- (9CI) (CA INDEX NAME)



RN 160115-23-1 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

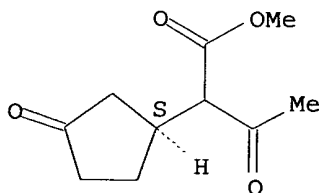
Absolute stereochemistry. Rotation (-).



RN 646038-06-4 HCAPLUS

CN Cyclopentaneacetic acid, α -acetyl-3-oxo-, methyl ester,
(1S)- (9CI) (CA INDEX NAME)

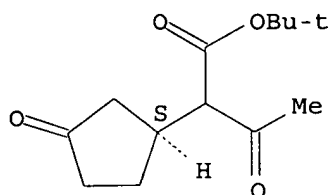
Absolute stereochemistry.



RN 708266-26-6 HCAPLUS

CN Cyclopentaneacetic acid, α -acetyl-3-oxo-, 1,1-dimethylethyl
ester, (1S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 24-4 (Alicyclic Compounds)

IT **Asymmetric synthesis and induction**

(asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

IT **Michael reaction**

Michael reaction catalysts

(stereoselective; asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

IT 195516-84-8 569336-64-7 569336-66-9

618912-25-7 709674-02-2 709674-03-3

RL: CAT (Catalyst use); USES (Uses)

(asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

IT 105-34-0, Methyl cyanoacetate 105-45-3, Methyl acetoacetate
108-59-8, Dimethyl malonate 123-54-6, Acetylacetone, reactions
626-35-7, Ethyl nitroacetate 930-30-3,
2-Cyclopenten-1-one 1694-31-1, tert-Butyl acetoacetate

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

IT 94410-50-1P 160115-23-1P 646038-06-4P

708266-26-6P 708266-27-7P 708266-28-8P

RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. Michael reactions of α -substituted acetates with cyclic enones catalyzed by multifunctional chiral Ru amido complexes)

REFERENCE COUNT: 37 THERE ARE 37 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 4 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2004:168607 HCAPLUS

DOCUMENT NUMBER: 140:357534

TITLE: Enantioselective Synthesis of (-)-Gilbertine
via a Cationic Cascade Cyclization

AUTHOR(S): Jiricek, Jan; Blechert, Siegfried

CORPORATE SOURCE: Institut fuer Chemie, Technische Universitaet
Berlin, Berlin, 10623, Germany

SOURCE: Journal of the American Chemical Society (
2004), 126(11), 3534-3538

CODEN: JACSAT; ISSN: 0002-7863

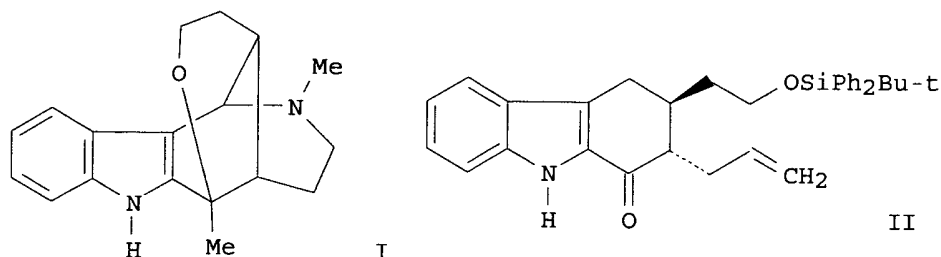
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 140:357534

GI



AB Described is the first enantioselective synthesis of (-)-gilbertine (I), a member of the uleine-type family, and the determination of the absolute configuration of this natural product is reported. The key step employs a cationic cascade reaction for a tetrahydropyran and piperidine ring formation and the construction of the pentacyclic framework in one step. The synthetic strategy utilizes the Shibasaki reaction to build up the first stereogenic center. A formylation reaction of a 3-substituted cyclohexanone derivative was achieved, giving only the desired regioisomer. The Japp-Klingemann Fischer indole protocol was used successfully as a convergent synthetic approach for the construction of the desired tetrahydrocarbazole (II). Furthermore, an unexpected behavior of this 2,3-disubstituted cyclohexanone derivative during an epimerization process was investigated, resulting in different chemical behavior of the enantiomers and the racemate. The diastereomeric resolution was achieved via the cationic cascade reaction, demonstrating the versatility of this approach. Significantly, the synthetic 17-step sequence was easy to execute, giving (-)-gilbertine in 5.5% overall yield.

ED Entered STN: 02 Mar 2004

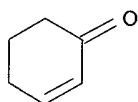
IT 930-68-7, 2-Cyclohexen-1-one

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 164931-77-5P 619329-97-4P

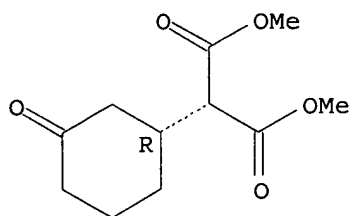
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)

RN 164931-77-5 HCAPLUS

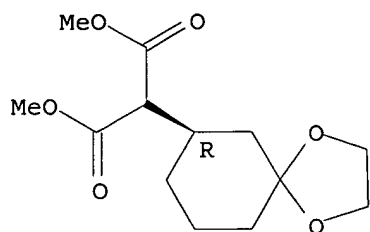
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 619329-97-4 HCAPLUS
CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.5]dec-7-yl-, dimethyl ester (9CI) (CA INDEX NAME)

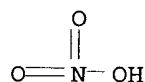
Absolute stereochemistry. Rotation (+).



CC 31-5 (Alkaloids)
IT **Asymmetric synthesis and induction**
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
IT 62-53-3, Aniline, reactions 106-95-6, Allyl bromide, reactions
108-59-8, Dimethyl malonate 109-94-4, Ethyl formate
930-68-7, 2-Cyclohexen-1-one 4229-44-1,
N-Methylhydroxylamine hydrochloride 681280-81-9
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
IT 71366-23-9P 85783-97-7P **164931-77-5P**
619329-97-4P 681280-63-7P 681280-64-8P 681280-65-9P
681280-66-0P 681280-67-1P 681280-68-2P 681280-71-7P
681280-72-8P 681280-73-9P 681280-74-0P 681280-75-1P
681280-76-2P 681280-78-4P 681280-79-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); **RACT (Reactant or reagent)**
(enantioselective synthesis of (-)-gilbertine via a cationic cascade cyclization)
REFERENCE COUNT: 34 THERE ARE 34 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 5 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:707973 HCAPLUS
DOCUMENT NUMBER: 139:307538
TITLE: Fe3+-exchanged fluorotetrasilicic mica as an
active and reusable catalyst for the Michael
reaction
AUTHOR(S): Shimizu, Ken-ichi; Miyagi, Masato; Kan-no,
Toshiki; Kodama, Tatsuya; Kitayama, Yoshie
CORPORATE SOURCE: Graduate School of Science and Technology,

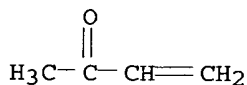
SOURCE: Niigata University, Niigata, 950-2181, Japan
Tetrahedron Letters (2003), 44(40),
7421-7424
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:307538
AB Fe³⁺-exchanged fluorotetrasilicic mica acts as a highly effective
and reusable catalyst for the solventless Michael reaction of
β-ketoesters with vinyl ketones under mild conditions. The
immobilized catalyst shows higher activity than homogeneous Fe³⁺
catalysts, FeCl₃·6H₂O and Fe(NO₃)₃·9H₂O.
ED Entered STN: 10 Sep 2003
IT 7782-61-8, Ferric nitrate nonahydrate
RL: CAT (Catalyst use); USES (Uses)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)
RN 7782-61-8 HCAPLUS
CN Nitric acid, iron(3+) salt, nonahydrate (9CI) (CA INDEX NAME)



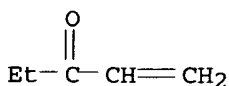
●1/3 Fe(III)

●3 H₂O

IT 78-94-4, 3-Buten-2-one, reactions 1629-58-9,
Ethyl vinyl ketone
RL: RCT (Reactant); RACT (Reactant or reagent)
(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)
RN 78-94-4 HCAPLUS
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



RN 1629-58-9 HCAPLUS
CN 1-Penten-3-one (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 28793-08-0P 31208-52-3P 35490-05-2P

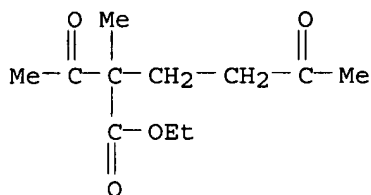
61771-80-0P 61771-81-1P 176101-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for Michael reaction of oxo esters with vinyl ketones)

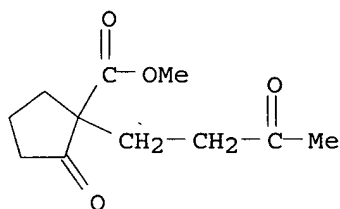
RN 28793-08-0 HCAPLUS

CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester (6CI, 8CI, 9CI) (CA INDEX NAME)



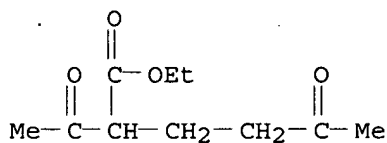
RN 31208-52-3 HCAPLUS

CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, methyl ester (8CI, 9CI) (CA INDEX NAME)



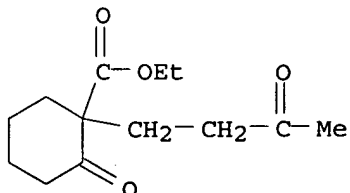
RN 35490-05-2 HCAPLUS

CN Hexanoic acid, 2-acetyl-5-oxo-, ethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)



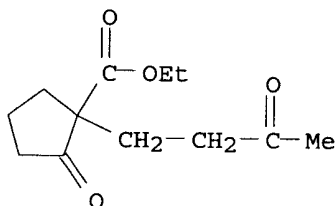
RN 61771-80-0 HCAPLUS

CN Cyclohexanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester (7CI, 9CI) (CA INDEX NAME)



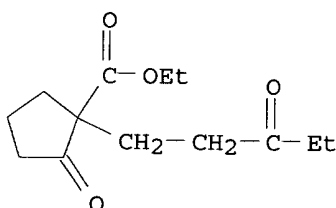
RN 61771-81-1 HCAPLUS

CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester
(6CI, 7CI, 9CI) (CA INDEX NAME)



RN 176101-58-9 HCAPLUS

CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxopentyl)-, ethyl ester
(9CI) (CA INDEX NAME)



CC 24-4 (Alicyclic Compounds)

Section cross-reference(s): 23

IT **Michael reaction catalysts**

(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)

IT 1318-93-0, Montmorillonite ((Al1.33-1.67Mg0.33-0.67)(Ca0-1Na0-1)0.33Si4(OH)2O10.xH2O), uses 7782-61-8, Ferric nitrate nonahydrate 10025-77-1, Ferric chloride hexahydrate 20074-52-6, Iron(3+), uses 56450-90-9, Fluorotetrasilicic mica
RL: CAT (Catalyst use); USES (Uses)

(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)

IT 78-94-4, 3-Buten-2-one, reactions 141-97-9, Ethyl acetoacetate 609-14-3, Ethyl 2-methylacetoacetate 611-10-9 1629-58-9, Ethyl vinyl ketone 1655-07-8 10472-24-9
RL: RCT (Reactant); RACT (Reactant or reagent)

(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)

IT 28793-08-0P 31208-52-3P 35490-05-2P
61771-80-0P 61771-81-1P 176101-58-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(iron(3+)-exchanged fluorotetrasilicic mica as catalyst for
Michael reaction of oxo esters with vinyl ketones)

REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 6 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:406901 HCAPLUS

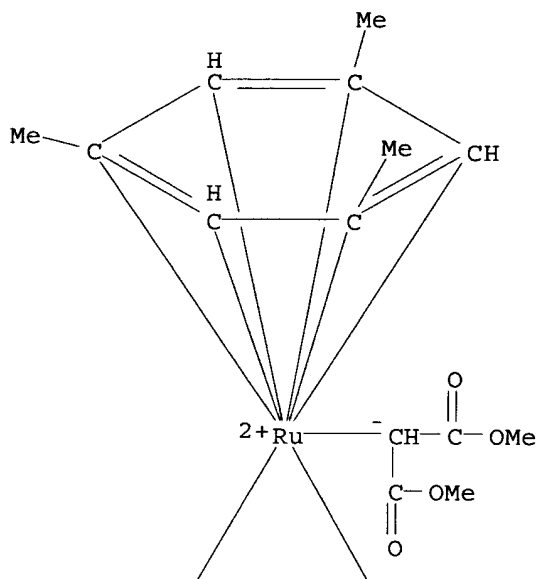
DOCUMENT NUMBER: 139:133131

TITLE: Enantioselective Michael Reaction Catalyzed by

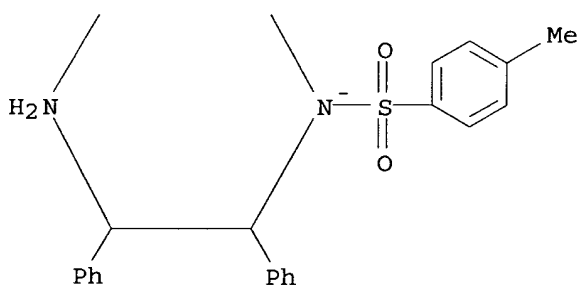
Well-Defined Chiral Ru Amido Complexes:
Isolation and Characterization of the Catalyst
Intermediate, Ru Malonato Complex Having a
Metal-Carbon Bond

AUTHOR(S): Watanabe, Masahito; Murata, Kunihiro; Ikariya,
Takao
CORPORATE SOURCE: Department of Applied Chemistry, Graduate
School of Science and Engineering, Tokyo
Institute of Technology and Frontier
Collaborative Research Center, Tokyo,
152-8552, Japan
SOURCE: Journal of the American Chemical Society (
2003), 125(25), 7508-7509
CODEN: JACSAT; ISSN: 0002-7863
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 139:133131
AB Chiral Ru amido complexes promote asym. Michael addition of malonates
to cyclic enones, leading to Michael adducts with excellent ee's,
in which the chiral Ru amido complexes react with malonates to
give isolable catalyst intermediates, chiral Ru malonato complexes
bearing a metal bound C-nucleophile.
ED Entered STN: 29 May 2003
IT 569336-67-0
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP
(Physical, engineering or chemical process); RCT (Reactant); FORM
(Formation, nonpreparative); PROC (Process); RACT (Reactant or
reagent)
(crystal structure of; enantioselective Michael reaction
catalyzed by well-defined chiral Ru amido complexes and
isolation and Ru malonato complex having metal-carbon bond
catalyst intermediate characterization)
RN 569336-67-0 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-
methylbenzenesulfonamido-κN][2-methoxy-1-(methoxycarbonyl)-
2-oxoethyl][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI)
(CA INDEX NAME)

PAGE 1-A

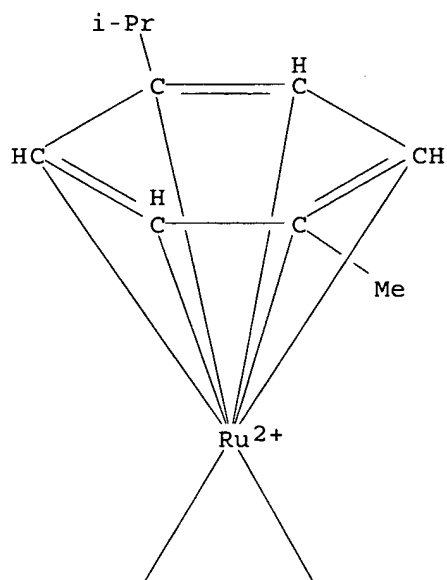


PAGE 2-A

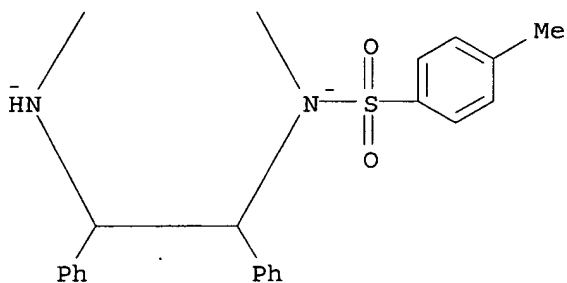


IT 195516-84-8 569336-63-6 569336-64-7
 569336-65-8 569336-66-9 618912-25-7
 RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical,
 engineering or chemical process); RCT (Reactant); PROC (Process);
 RACT (Reactant or reagent); USES (Uses)
 (enantioselective Michael reaction catalyzed by well-defined
 chiral Ru amido complexes and isolation and Ru malonato complex
 having metal-carbon bond catalyst intermediate
 characterization)
 RN 195516-84-8 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-
 methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1-
 methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

PAGE 1-A



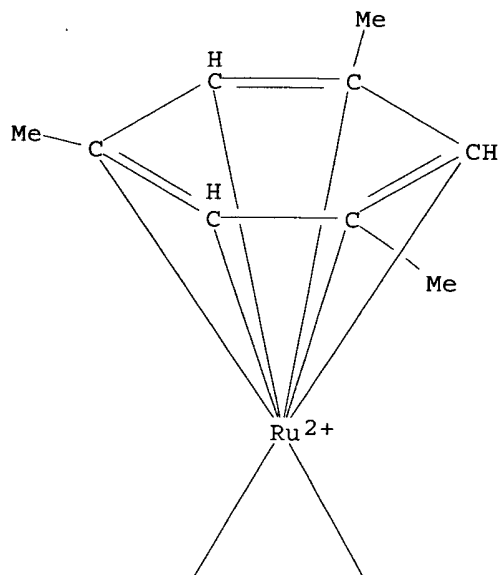
PAGE 2-A



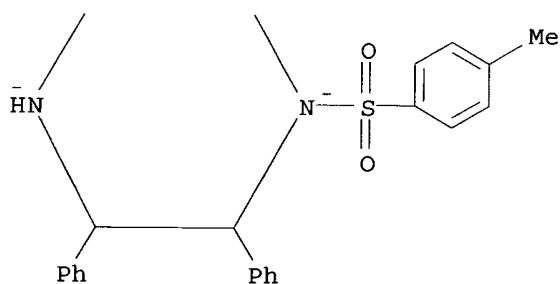
RN 569336-63-6 HCAPLUS

CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamidato(2-)-κN][(1,2,3,4,5,6-η)-1,3,5-trimethylbenzene]- (9CI) (CA INDEX NAME)

PAGE 1-A

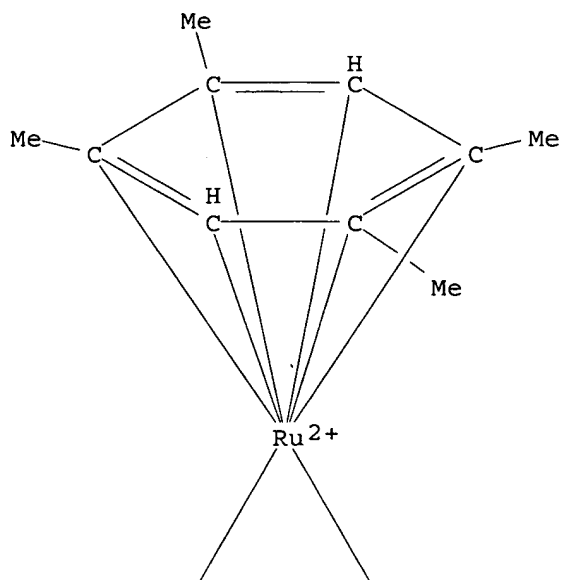


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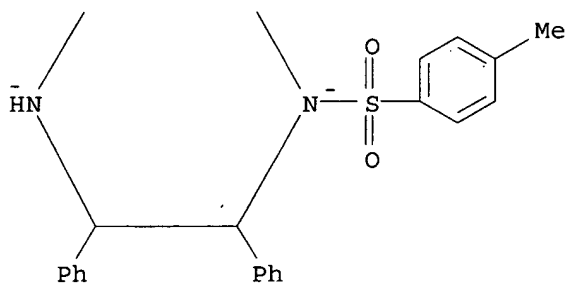


RN 569336-64-7 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-1,2,4,5-tetramethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

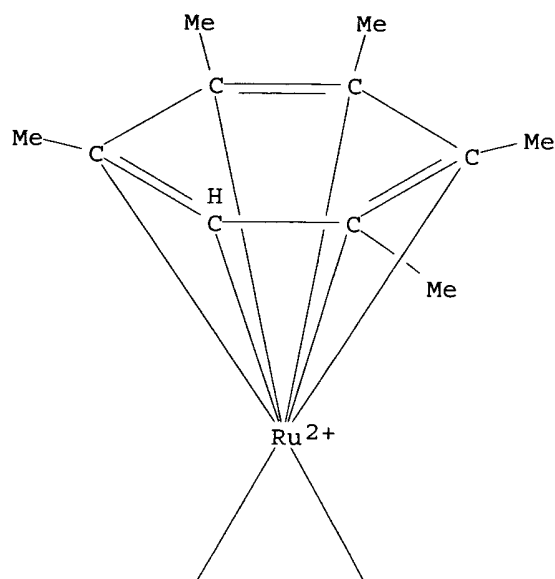


PAGE 2-A

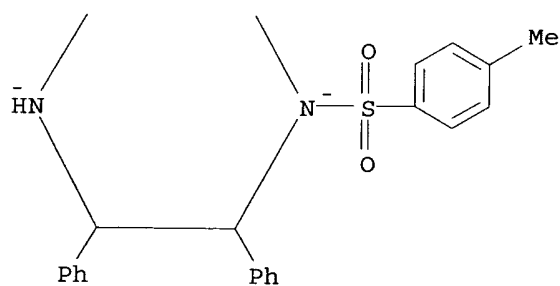


RN 569336-65-8 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-pentamethylbenzene]-(9CI) (CA INDEX NAME)

PAGE 1-A

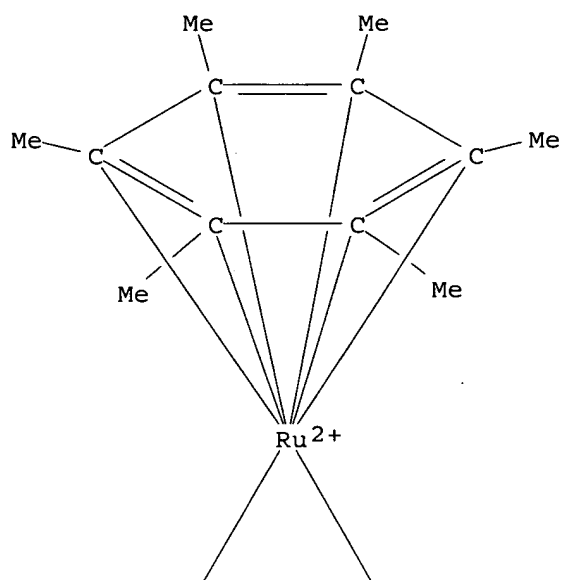


PAGE 2-A

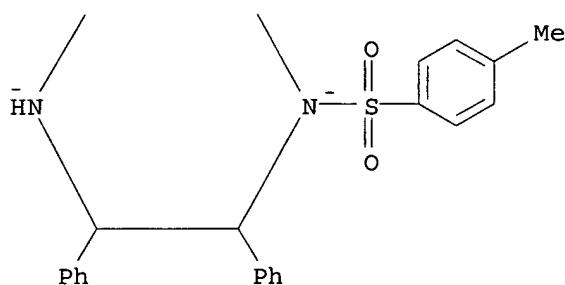


RN 569336-66-9 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-(amino-κN)-1,2-diphenylethyl]-4-methylbenzenesulfonamido(2-)-κN][(1,2,3,4,5,6-η)-hexamethylbenzene]-(9CI) (CA INDEX NAME)

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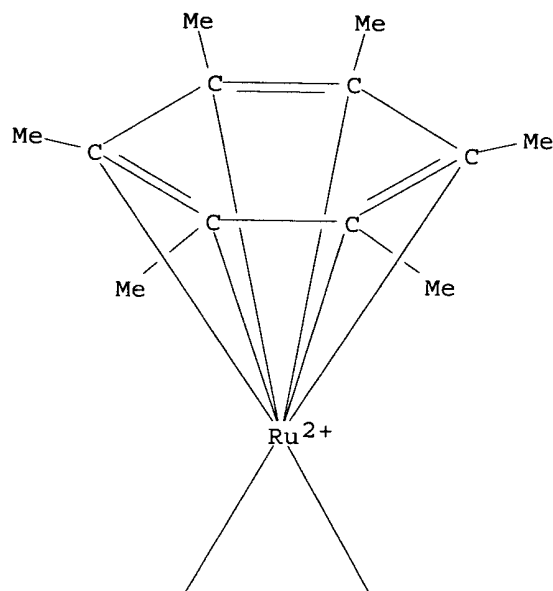


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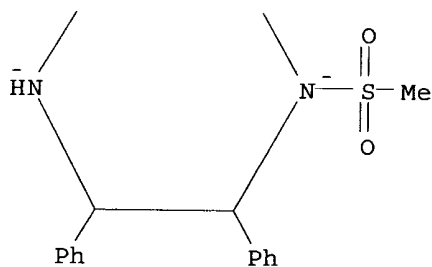


RN 618912-25-7 HCAPLUS
 CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]methanesulfonamid
 ato(2-)-κN] [(1,2,3,4,5,6-η)-hexamethylbenzene] - (9CI)
 (CA INDEX NAME)

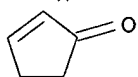
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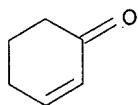
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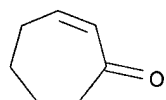
IT 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone
 22748-16-9, 4,4-Dimethyl-2-cyclopentenone
 RL: CPS (Chemical process); PEP (Physical, engineering or chemical
 process); RCT (Reactant); PROC (Process); **RACT (Reactant or
 reagent)**
 (enantioselective Michael reaction catalyzed by well-defined
 chiral Ru amido complexes and isolation and Ru malonato complex
 having metal-carbon bond catalyst intermediate
 characterization)
 RN 930-30-3 HCAPLUS
 CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



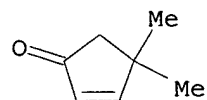
RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

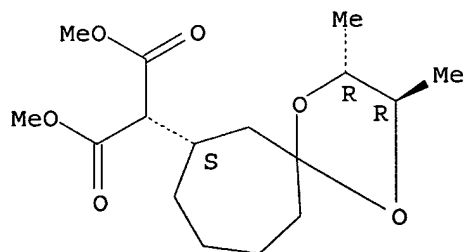


RN 22748-16-9 HCAPLUS
CN 2-Cyclopenten-1-one, 4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



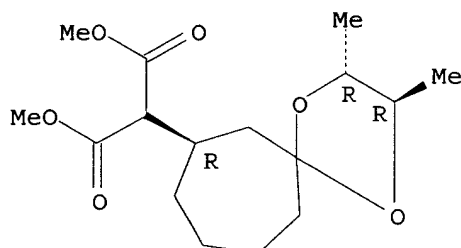
IT 569342-28-5 569342-29-6
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
RN 569342-28-5 HCAPLUS
CN Propanedioic acid, [(2R,3R,7S)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



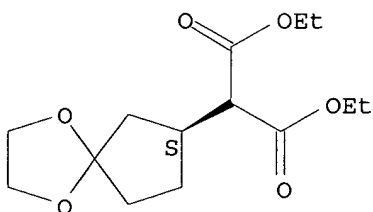
RN 569342-29-6 HCAPLUS
 CN Propanedioic acid, [(2R,3R,7R)-2,3-dimethyl-1,4-dioxaspiro[4.6]undec-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

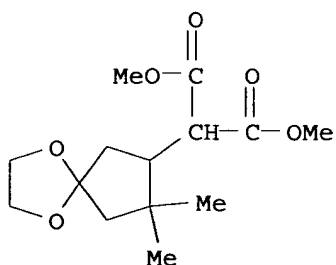


IT 193530-88-0 568590-07-8
 RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
 (enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
 RN 193530-88-0 HCAPLUS
 CN Propanedioic acid, (7S)-1,4-dioxaspiro[4.4]non-7-yl-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 568590-07-8 HCAPLUS
 CN Propanedioic acid, (8,8-dimethyl-1,4-dioxaspiro[4.4]non-7-yl)-, dimethyl ester (9CI) (CA INDEX NAME)



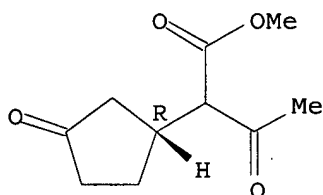
IT 568590-08-9P

RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent) (enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 568590-08-9 HCAPLUS

CN Cyclopentaneacetic acid, α -acetyl-3-oxo-, methyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 154194-50-0P 160115-23-1P 568590-05-6P

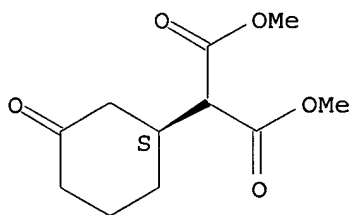
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)

(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

RN 154194-50-0 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

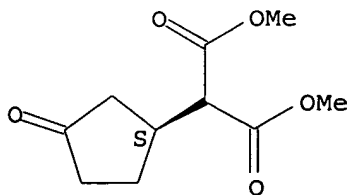
Absolute stereochemistry. Rotation (-).



RN 160115-23-1 HCAPLUS

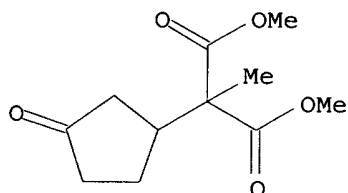
CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



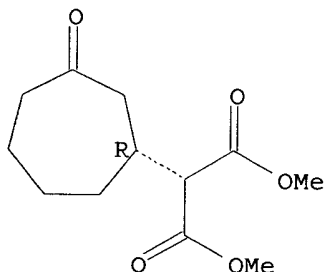
RN 568590-05-6 HCAPLUS
 CN Propanedioic acid, methyl(3-oxocyclopentyl)-, dimethyl ester, (-)-(9CI) (CA INDEX NAME)

Rotation (-).



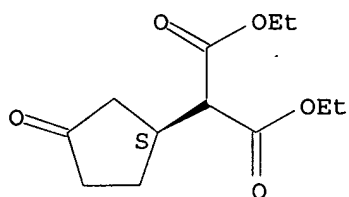
IT 287493-82-7
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (enantioselective Michael reaction catalyzed by well-defined
 chiral Ru amido complexes and isolation and Ru malonato complex
 having metal-carbon bond catalyst intermediate
 characterization)
 RN 287493-82-7 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



IT 193530-87-9P 568590-04-5P 568590-06-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (enantioselective Michael reaction catalyzed by well-defined
 chiral Ru amido complexes and isolation and Ru malonato complex
 having metal-carbon bond catalyst intermediate
 characterization)
 RN 193530-87-9 HCAPLUS
 CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
 (CA INDEX NAME)

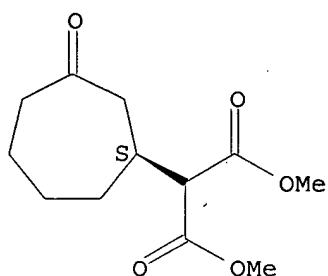
Absolute stereochemistry. Rotation (-).



RN 568590-04-5 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocycloheptyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

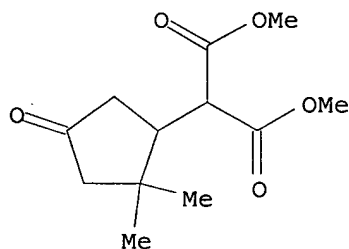
Absolute stereochemistry.



RN 568590-06-7 HCAPLUS

CN Propanedioic acid, (2,2-dimethyl-4-oxocyclopentyl)-, dimethyl ester, (-)- (9CI) (CA INDEX NAME)

Rotation (-).



CC 22-3 (Physical Organic Chemistry)
Section cross-reference(s): 29, 75

IT **Asymmetric synthesis and induction**
Stereochemistry

Transition state structure

(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

IT **Michael reaction**

Michael reaction catalysts

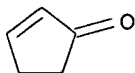
(stereoselective; enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

- IT 569336-67-0
RL: CPS (Chemical process); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process); RACT (Reactant or reagent)
(crystal structure of; enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 195516-84-8 569336-63-6 569336-64-7
569336-65-8 569336-66-9 618912-25-7
RL: CAT (Catalyst use); CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); RACT (Reactant or reagent); USES (Uses)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 105-45-3, Methyl acetylacetate 105-53-3, Diethyl malonate
108-59-8, Dimethyl malonate 609-02-9, Dimethyl methylmalonate
930-30-3, 2-Cyclopentenone 930-68-7, 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone
22748-16-9, 4,4-Dimethyl-2-cyclopentenone
RL: CPS (Chemical process); PEP (Physical, engineering or chemical process); RCT (Reactant); PROC (Process); **RACT (Reactant or reagent)**
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 84308-31-6 569342-28-5 569342-29-6
RL: FMU (Formation, unclassified); FORM (Formation, nonpreparative)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 193530-88-0 568590-07-8
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PYP (Physical process); FORM (Formation, nonpreparative); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 568590-08-9P
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)
- IT 154194-50-0P 160115-23-1P 568590-05-6P
RL: PEP (Physical, engineering or chemical process); PYP (Physical process); SPN (Synthetic preparation); PREP (Preparation); PROC (Process)
(enantioselective Michael reaction catalyzed by well-defined chiral Ru amido complexes and isolation and Ru malonato complex having metal-carbon bond catalyst intermediate characterization)

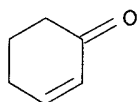
characterization)
IT 126-39-6, 2-Ethyl-2-methyl-1,3-dioxolane 287493-82-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined
chiral Ru amido complexes and isolation and Ru malonato complex
having metal-carbon bond catalyst intermediate
characterization)
IT 193530-87-9P 568590-04-5P 568590-06-7P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(enantioselective Michael reaction catalyzed by well-defined
chiral Ru amido complexes and isolation and Ru malonato complex
having metal-carbon bond catalyst intermediate
characterization)

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 7 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 2003:315962 HCAPLUS
DOCUMENT NUMBER: 140:76842
TITLE: Effect of microwaves in the chiral switching
asymmetric Michael reaction
AUTHOR(S): Narasimhan, S.; Velmathi, S.
CORPORATE SOURCE: Centre for Natural Products, SPIC Science
Foundation, Guindy, Chennai, 600 032, India
SOURCE: Molecules (2003), 8(2), 256-262
CODEN: MOLEFW; ISSN: 1420-3049
URL: <http://www.mdpi.org/molecules/papers/80200256.pdf>
PUBLISHER: Molecular Diversity Preservation International
DOCUMENT TYPE: Journal; (online computer file)
LANGUAGE: English
OTHER SOURCE(S): CASREACT 140:76842
AB Highly enantioselective Michael reactions of malonates with cyclic
enones are achieved in remarkably less time under microwave
irradiation using newly developed heterobimetallic catalysts.
ED Entered STN: 24 Apr 2003
IT 930-30-3, 2-Cyclopenten-1-one 930-68-7,
2-Cyclohexen-1-one
RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael addition reaction of cyclic enones with
malonates utilizing chiral heterobimetallic catalyst system
under microwave irradiation)
RN 930-30-3 HCAPLUS
CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 151600-50-9P 164931-78-6P 177722-18-8P

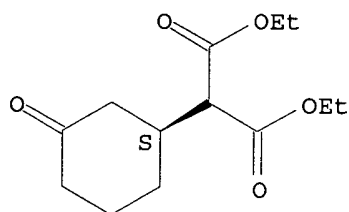
193530-87-9P 334699-04-6P 334699-05-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition reaction of cyclic enones with
malonates utilizing chiral heterobimetallic catalyst system
under microwave irradiation)

RN 151600-50-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

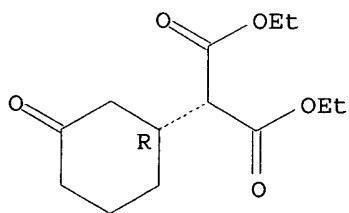
Absolute stereochemistry. Rotation (-).



RN 164931-78-6 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

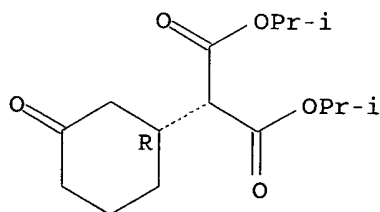
Absolute stereochemistry. Rotation (+).



RN 177722-18-8 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1-methylethyl)
ester (9CI) (CA INDEX NAME)

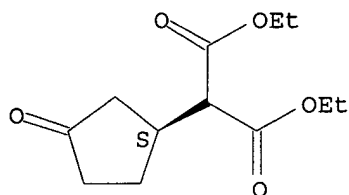
Absolute stereochemistry. Rotation (+).



RN 193530-87-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

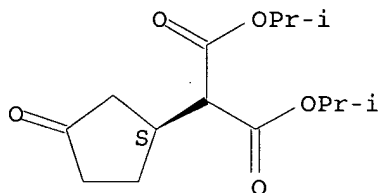
Absolute stereochemistry. Rotation (-).



RN 334699-04-6 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, bis(1-methylethyl)
ester (9CI) (CA INDEX NAME)

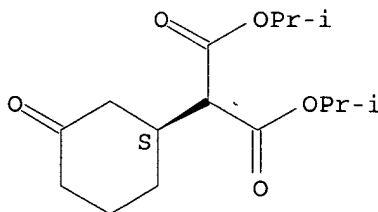
Absolute stereochemistry. Rotation (-).



RN 334699-05-7 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, bis(1-methylethyl)
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 23

IT **Asymmetric synthesis and induction**

(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

IT Addition reaction catalysts

Michael reaction

(stereoselective; enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

IT 105-53-3, Ethyl malonate 930-30-3, 2-Cyclopenten-1-one
930-68-7, 2-Cyclohexen-1-one 13195-64-7, Diisopropyl

malonate 15014-25-2, Dibenzyl malonate

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

IT 151600-50-9P 154194-47-5P 154194-49-7P 164931-75-3P

164931-78-6P 177722-18-8P 193530-87-9P

334699-04-6P 334699-05-7P

RL: SPN (Synthetic preparation); PREP (Preparation)

(enantioselective Michael addition reaction of cyclic enones with malonates utilizing chiral heterobimetallic catalyst system under microwave irradiation)

REFERENCE COUNT: 23 THERE ARE 23 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 8 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:160178 HCAPLUS

DOCUMENT NUMBER: 139:36248

TITLE: Highly enantioselective organocatalytic conjugate addition of malonates to acyclic α,β -unsaturated enones

AUTHOR(S): Halland, Nis; Aburel, Pompiliu S.; Jorgensen, Karl Anker

CORPORATE SOURCE: Danish National Research Foundation: Center for Catalysis Department of Chemistry, Aarhus University, Aarhus C, 8000, Den.

SOURCE: Angewandte Chemie, International Edition (2003), 42(6), 661-665

CODEN: ACIEF5; ISSN: 1433-7851

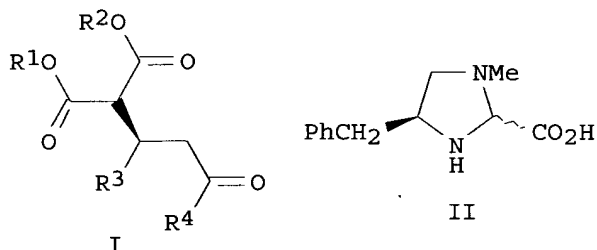
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:36248

GI



AB We have developed the first highly enantioselective selective organocatalytic Michael addition of malonates R1O2CCH2CO2R2 (R1 = R2 = Me, Et, CHMe2, CMe3, allyl, CH2Ph; R1 = CH2Ph, R2 = Me, Et; R1 = Et, R2 = CMe3) to α,β -unsatd. enones R3CH:CHCOR4 [R3 = Ph, 2-naphthyl, 4-ClC6H4, 4-HOC6H4, etc., R4 = Me; R3R4 = (CH2)3; R3 = Ph, R4 = Et, CHMe2] to offer adducts I using an imidazolidine catalyst II easily prepared from phenylalanine. The scope of the reaction is demonstrated by the synthesis of optically active δ keto esters, e.g. Me (3R)-5-oxo-3-phenylhexanoate, and

tetrahydroquinolines, such as (2R,4R)-2-methyl-4-bis(methoxycarbonyl)methyltetrahydroquinoline.

ED Entered STN: 04 Mar 2003

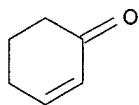
IT 930-68-7, 2-Cyclohexen-1-one 5166-53-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)

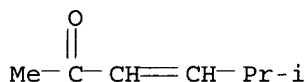
RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 5166-53-0 HCAPLUS

CN 3-Hexen-2-one, 5-methyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 109012-81-9P 196399-49-2P

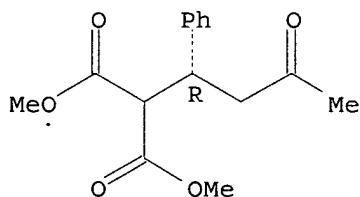
RL: SPN (Synthetic preparation); PREP (Preparation)

(enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)

RN 109012-81-9 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxo-1-phenylbutyl]-, dimethyl ester (9CI) (CA INDEX NAME)

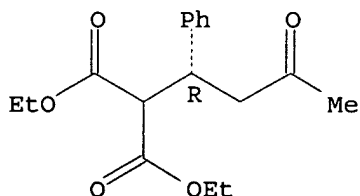
Absolute stereochemistry.



RN 196399-49-2 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxo-1-phenylbutyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 23-17 (Aliphatic Compounds)
IT **Asymmetric synthesis and induction**
(enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)
IT 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate
122-57-6, Benzylideneacetone 623-15-4 874-83-9
930-68-7, 2-Cyclohexen-1-one 1669-44-9, 3-Octen-2-one
1797-75-7 3152-68-9 3160-32-5 3160-35-8 3160-40-5
3490-37-7 4188-88-9 **5166-53-0** 5432-53-1 13195-64-7
15014-25-2, Dibenzyl malonate 20766-40-9 32864-38-3
42998-51-6 52267-39-7 61453-86-9 75032-63-2 89393-74-8
RL: RCT (Reactant); **RAC** (Reactant or reagent)
(enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)
IT **109012-81-9P** 164931-75-3P **196399-49-2P**
541508-71-8P 541508-72-9P 541508-73-0P 541508-74-1P
541508-75-2P 541508-76-3P 541508-77-4P 541508-78-5P
541508-79-6P 541508-80-9P 541508-81-0P 541508-82-1P
541508-83-2P 541508-84-3P 541508-85-4P 541508-86-5P
541508-87-6P 541508-88-7P 541508-89-8P 541508-90-1P
RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael addition of malonates to acyclic α,β -unsatd. enones with imidazolidine catalyst)
REFERENCE COUNT: 57 THERE ARE 57 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 9 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:110333 HCAPLUS

DOCUMENT NUMBER: 138:287306

TITLE: Catalysis of the Michael Addition Reaction by
Late Transition Metal Complexes of
BINOL-Derived Salens

AUTHOR(S): Annamalai, Venkatachalam; DiMauro, Erin F.;
Carroll, Patrick J.; Kozlowski, Marisa C.

CORPORATE SOURCE: Department of Chemistry, Roy and Diana Vagelos
Laboratories, University of Pennsylvania,
Philadelphia, PA, 19104-6323, USA

SOURCE: Journal of Organic Chemistry (2003),
68(5), 1973-1981
CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:287306

AB Salen metal complexes incorporating two chiral BINOL moieties have been synthesized and characterized by X-ray crystallog. The X-ray structures show that this new class of Ni-BINOL-salen catalysts contains an unoccupied apical site for potential coordination of an electrophile and naphthoxides that are independent from the Lewis acid center. These characteristics allow independent alteration of the Lewis acidic and Bronsted basic sites. These unique complexes have been shown to catalyze the Michael reaction of dibenzyl malonate and cyclohexenone with good selectivity (up to 90% ee) and moderate yield (up to 79% yield). These catalysts

are also effective in the Michael reaction between other enones and malonates. Kinetic data show that the reaction is first order in the Ni-Cs-BINOL-salen catalyst. Further expts. probed the reactivity of the individual Lewis acid and Bronsted base components of the catalyst and established that both moieties are essential for asym. catalysis. All told, the data support a bifunctional activation pathway in which the apical Ni site of the Ni-Cs-BINOL-salen activates the enone and the naphthoxide base activates the malonate.

ED Entered STN: 13 Feb 2003

IT 930-30-3, 2-Cyclopentenone 930-68-7,

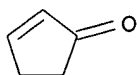
2-Cyclohexenone 1121-66-0, 2-Cycloheptenone

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

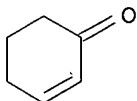
RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



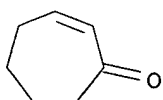
RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS

CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



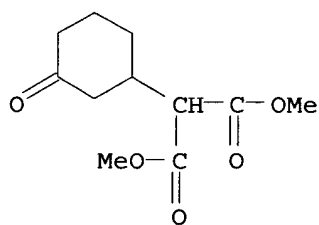
IT 33646-18-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

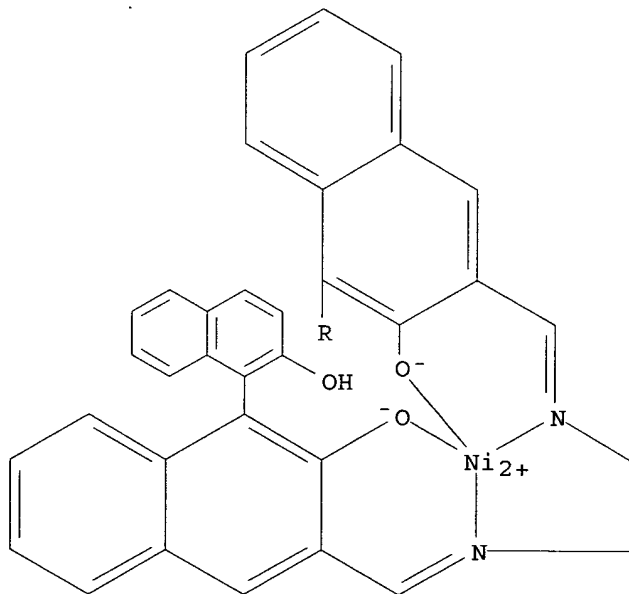
RN 33646-18-3 HCAPLUS

CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)

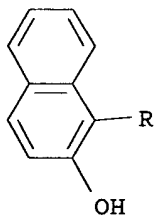


IT 349140-08-5P 349149-15-1P
 RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
 PREP (Preparation); RACT (Reactant or reagent)
 (preparation and crystal structure of nickel BINOL-derived
 salen-type catalysts for Michael addition reaction)
 RN 349140-08-5 HCAPLUS
 CN Nickel, [[(1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-
 κ N)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κ O2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

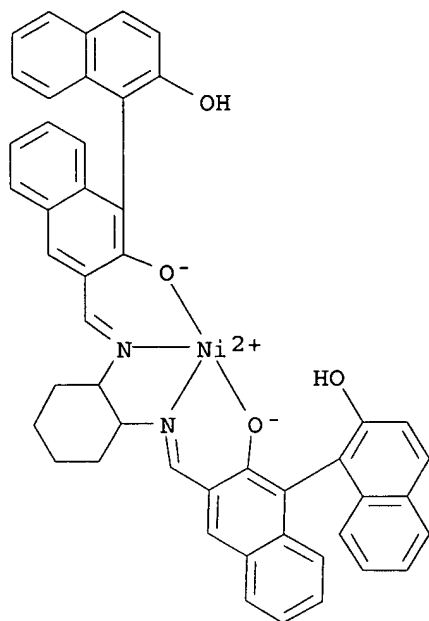
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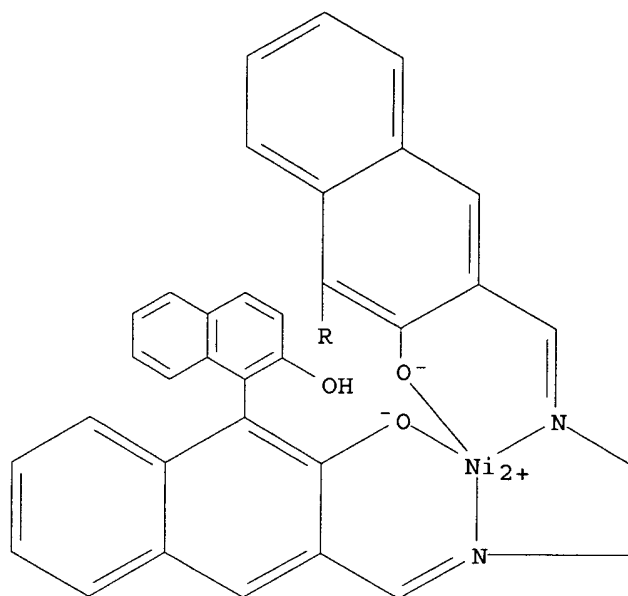


RN 349149-15-1 HCAPLUS
 CN Nickel, [[[1S,1''S)-3,3''-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-
 κ N)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κ O2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

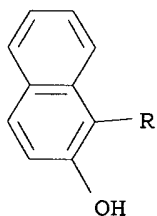


IT 349140-17-6P 349140-18-7P 349149-18-4P
 504394-83-6P 504409-95-4P 504410-02-0P
 504410-04-2P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
 (Preparation); USES (Uses)
 (preparation of nickel BINOL-derived salen-type catalysts for
 Michael addition reaction)
 RN 349140-17-6 HCAPLUS
 CN Nickelate(2-), [[[1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-
 κ N)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κ O2]](4-)]-, dicesium, (SP-4-2)- (9CI) (CA INDEX NAME)

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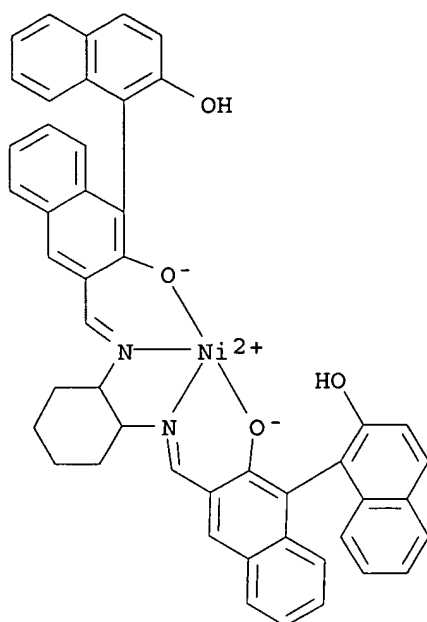


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● 2 Cs

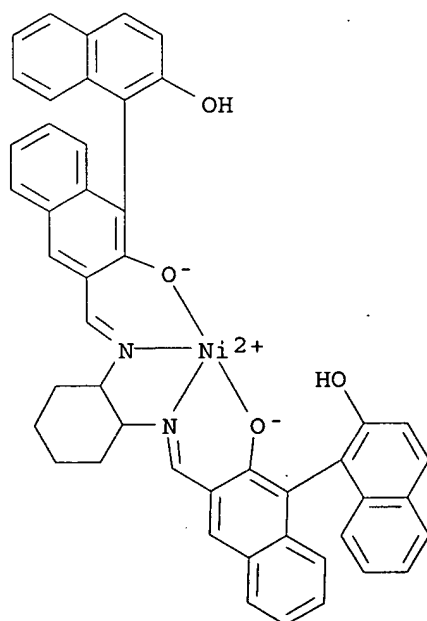
RN 349140-18-7 HCAPLUS
 CN Nickelate(2-), [[[(1S,1''S)-3,3''-[(1S,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](4-)]-, dicesium, (SP-4-2)-(9CI) (CA INDEX NAME)



● 2 Cs

RN 349149-18-4 HCAPLUS

CN Nickelate(2-), [[(1S,1''S)-3,3''-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](4-)]-, dicesium, (SP-4-2)-(9CI) (CA INDEX NAME)

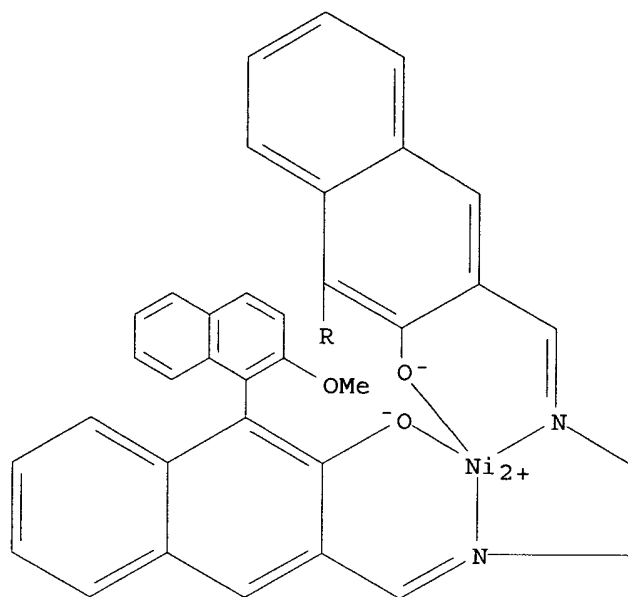


● 2 Cs

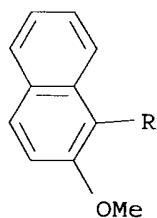
RN 504394-83-6 HCAPLUS

CN Nickel, [[(1S,1''S)-3,3''-[1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[2'-methoxy[1,1'-binaphthalen]-2-olato-κO]](2-)]-, (SP-4-2)-(9CI) (CA INDEX NAME)

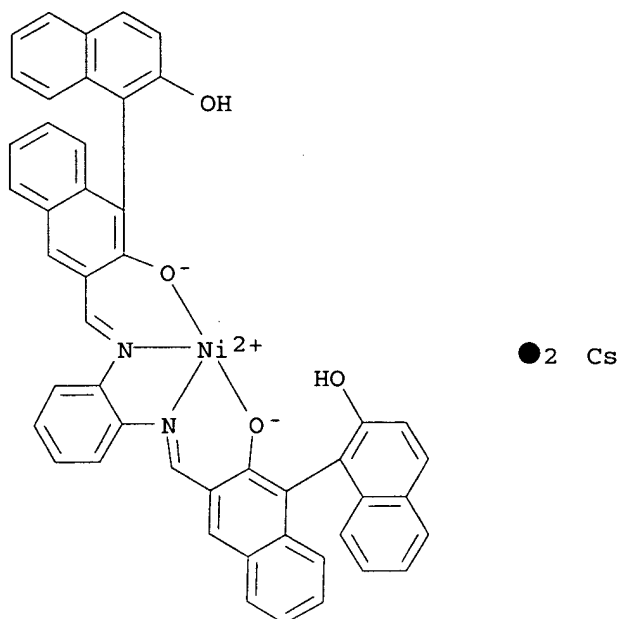
PAGE 1-A



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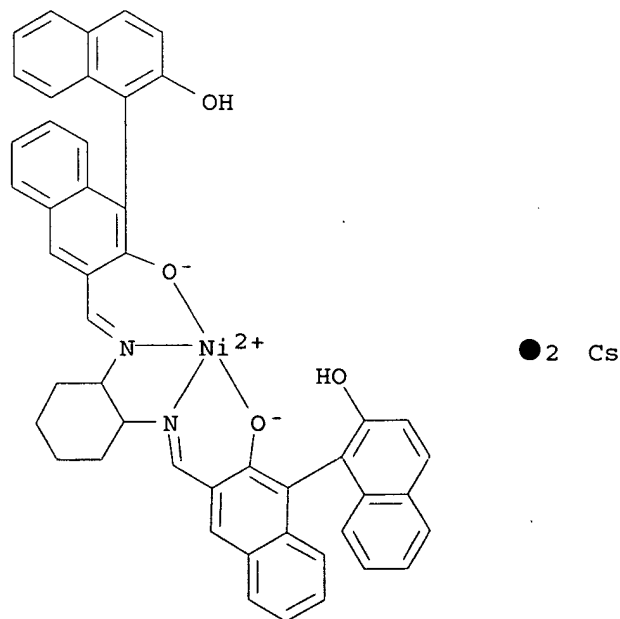


RN 504409-95-4 HCAPLUS
 CN Nickel, [[(1S,1''S)-3,3''-[1,2-phenylenebis[(nitrilo-
 κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κO2]](2-)]-, dicesium salt, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 504410-02-0 HCAPLUS

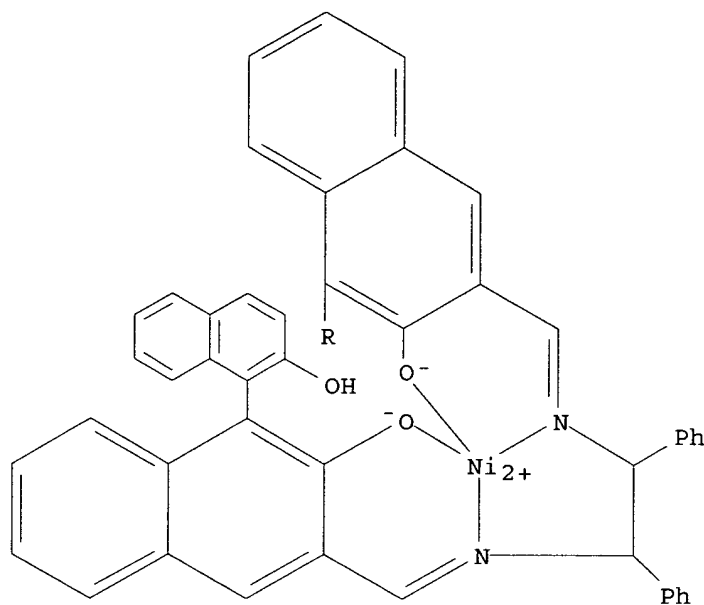
CN Nickel, [[[1S,1''S)-3,3''-[(1R,2S)-1,2-cyclohexanediyl]bis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, dicesium salt, (SP-4-4)- (9CI) (CA INDEX NAME)



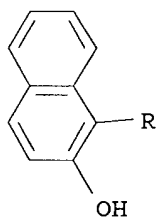
RN 504410-04-2 HCAPLUS

CN Nickel, [[[1S,1''S)-3,3''-[[[(1R,2R)-1,2-diphenyl-1,2-ethanediyl]bis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, dicesium salt, (SP-4-2)- (9CI) (CA INDEX NAME)

PAGE 1-A

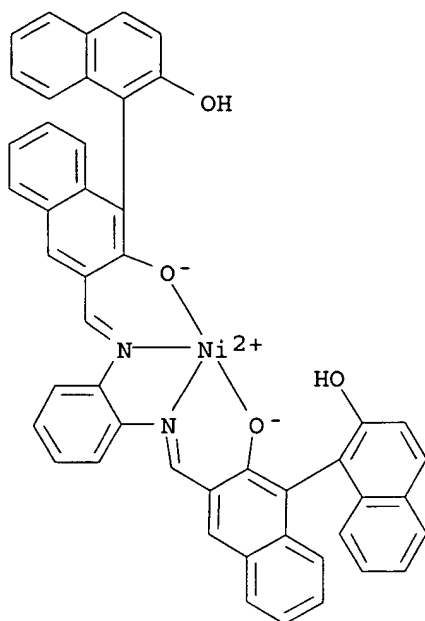


PAGE 2-A



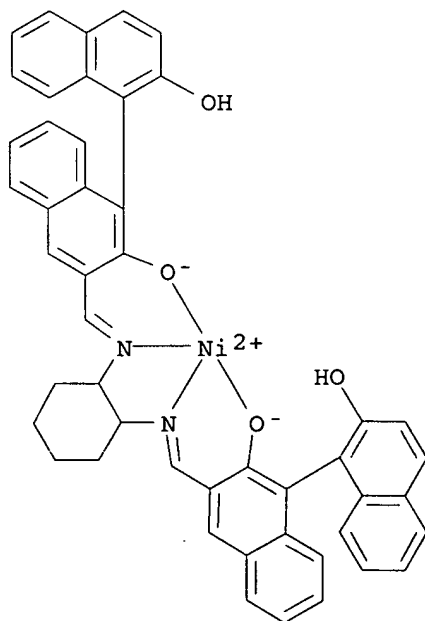
● 2 Cs

IT 349140-12-1P 349140-14-3P 349140-16-5P
 349149-17-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation of nickel BINOL-derived salen-type catalysts for
 Michael addition reaction)
 RN 349140-12-1 HCAPLUS
 CN Nickel, [[[1S,1''S)-3,3''-[1,2-phenylenebis[(nitrilo-
 κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



RN 349140-14-3 HCAPLUS

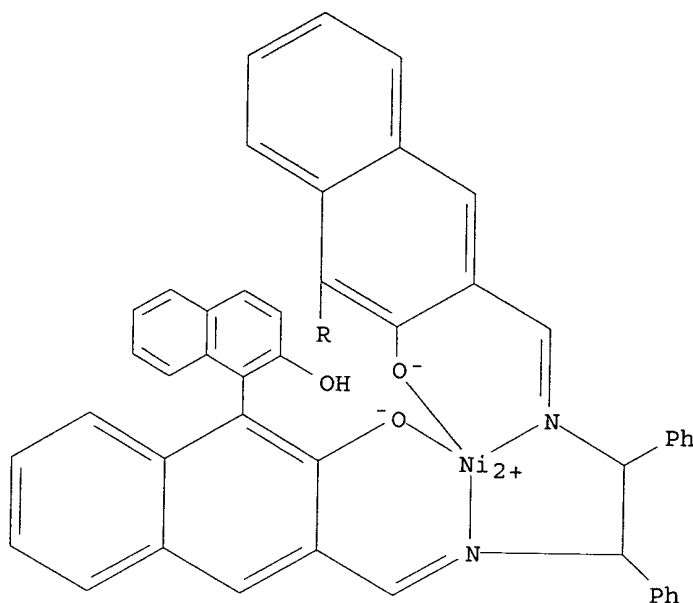
CN Nickel, [[[1S,1''S)-3,3''-[(1S,2S)-1,2-cyclohexanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



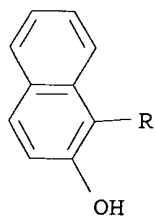
RN 349140-16-5 HCAPLUS

CN Nickel, [[[1S,1''S)-3,3''-[[[(1R,2R)-1,2-diphenyl-1,2-ethanediylbis[(nitrilo-κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)

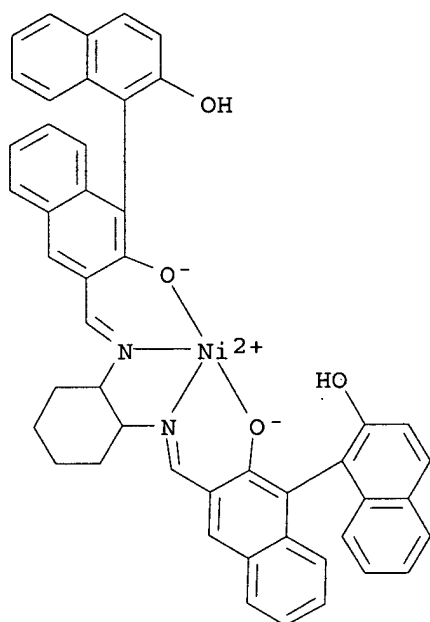
PAGE 1-A



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RN 349149-17-3 HCAPLUS
 CN Nickel, [[[1S,1''S)-3,3''-[(1R,2S)-1,2-cyclohexanediylbis[(nitrilo-
 κN)methylidyne]]bis[[1,1'-binaphthalene]-2,2'-diolato-
 κO2]](2-)]-, (SP-4-4)- (9CI) (CA INDEX NAME)

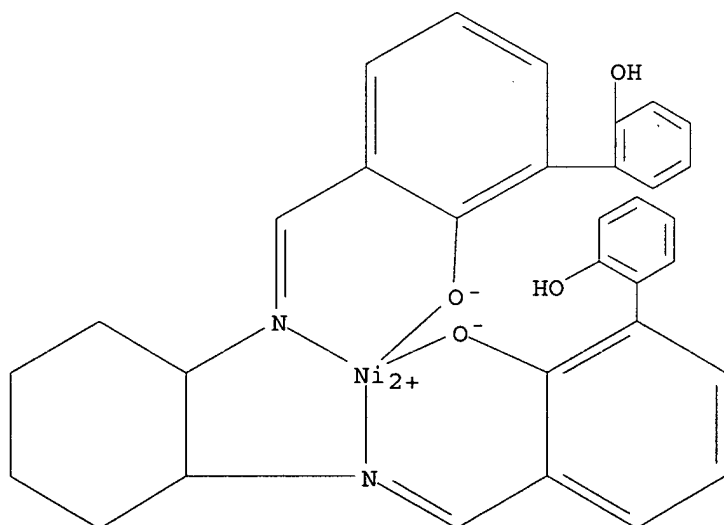


IT 504394-80-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of nickel BINOL-derived salen-type catalysts for
Michael addition reaction)

RN 504394-80-3 HCAPLUS

CN Nickel, [[3,3'-[(1R,2R)-1,2-cyclohexanediylbis[(nitrilo-
κN)methylidyne]]bis[[1,1'-biphenyl]-2,2'-diolato-
κO2]](2-)]-, (SP-4-2)- (9CI) (CA INDEX NAME)



CC 24-5 (Alicyclic Compounds)

Section cross-reference(s): 25, 78

IT Michael reaction

Michael reaction catalysts

(stereoselective; catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT 108-59-8, Dimethyl malonate 614-47-1, trans-Chalcone 930-30-3, 2-Cyclopentenone 930-68-7, 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone 5153-67-3, trans- β -Nitrostyrene 15014-25-2, Dibenzyl malonate

RL: RCT (Reactant); RACT (Reactant or reagent)

(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT 33646-18-3P 55790-16-4P 67488-98-6P 164931-75-3P 181712-81-2P 504394-81-4P 504394-82-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(catalysis of the Michael addition reaction by late transition metal complexes of BINOL-derived salens)

IT 349140-08-5P 349149-15-1P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and crystal structure of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT 349140-17-6P 349140-18-7P 349149-18-4P 504394-83-6P 504409-95-4P 504410-02-0P 504410-04-2P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT 156660-22-9P, 2,2'-Dihydroxy-1,1'-biphenyl-3-carboxaldehyde 209908-74-7P 349140-12-1P 349140-14-3P 349140-16-5P 349149-09-3P 349149-10-6P 349149-11-7P 349149-12-8P 349149-13-9P 349149-14-0P 349149-17-3P 504394-79-0P 504407-87-8P 504407-88-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

IT 504394-80-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of nickel BINOL-derived salen-type catalysts for Michael addition reaction)

REFERENCE COUNT: 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 10 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2003:67244 HCAPLUS

DOCUMENT NUMBER: 139:6420

TITLE: Novel heterobimetallic catalysts for asymmetric Michael reactions

AUTHOR(S): Velmathi, S.; Swarnalakshmi, S.; Narasimhan, S.

CORPORATE SOURCE: T.R. Govindachari Centre for Natural Products, SPIC Science Foundation, Chennai, 600 032, India

SOURCE: Tetrahedron: Asymmetry (2003), 14(1), 113-117

CODEN: TASYE3; ISSN: 0957-4166

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:6420

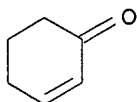
AB The newly developed chiral catalysts based on organoborane and organoaluminum complexes show opposite enantioselectivity in Michael addition reactions of cyclic enones and malonates resulting in the production of both enantiomers of products in good chemical yield and enantiomeric excess. ²⁷Al NMR studies showed the formation of different types of complexes for these catalysts and the enantioselectivity was found to be dependent on the nature of the aluminum complex formed. Scope of the reaction was extended to other Michael donors such as nitro alkanes and thiols.

ED Entered STN: 29 Jan 2003

IT 930-68-7, 2-Cyclohexenone
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

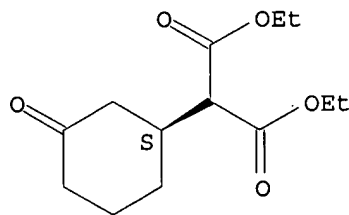


IT 151600-50-9P 164931-78-6P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition reactions of cyclic enones and malonates in presence of organoaluminum and organoborane complex catalysts)

RN 151600-50-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

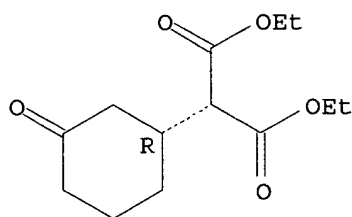
Absolute stereochemistry. Rotation (-).



RN 164931-78-6 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

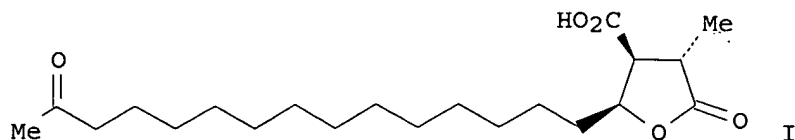
Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)
 IT **Asymmetric synthesis and induction**
 (of cyclohexane malonates and acyclic α,β -unsatd.
 enones and enols in presence of organoaluminum and organoborane
 complexes)
 IT **Michael reaction**
 (stereoselective; of cyclohexanone with di-Et malonate and
 malonic esters, nitro alkanes, and thiols in presence of
 organoaluminum and organoborane complex **catalysts**)
 IT **Michael reaction catalysts**
 (stereoselective; organoaluminum and organoborane complex
 catalysts for asym. Michael addition of cyclohexanone with di-Et
 malonate and malonic esters, nitro alkanes, and thiols)
 IT 105-53-3, Diethyl malonate **930-68-7**, 2-Cyclohexenone
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (asym. Michael addition reactions of cyclic enones and malonates
 in presence of organoaluminum and organoborane complex
 catalysts)
 IT **151600-50-9P 164931-78-6P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. Michael addition reactions of cyclic enones and malonates
 in presence of organoaluminum and organoborane complex
 catalysts)

REFERENCE COUNT: 26 THERE ARE 26 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L93 ANSWER 11 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2003:4446 HCAPLUS
 DOCUMENT NUMBER: 138:237913
 TITLE: Synthesis of (\pm)-nephromopsinic,
 (-)-phaseolinic, and (-)-dihydropertusaric
 acids
 AUTHOR(S): Brecht-Forster, Andrea; Fitremann, Juliette;
 Renaud, Philippe
 CORPORATE SOURCE: Universite de Fribourg, Departement de Chimie,
 Fribourg, CH-1700, Switz.
 SOURCE: Helvetica Chimica Acta (2002),
 85(11), 3965-3974
 CODEN: HCACAV; ISSN: 0018-019X
 PUBLISHER: Verlag Helvetica Chimica Acta
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:237913
 GI



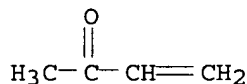
AB The formal syntheses of (±)-nephromopsinic acid, (-)-phaseolinic acid, and the first total synthesis of (-)-dihydropertusaric acid (I) from (±)- and (-)-7-oxabicyclo[2.2.1]hept-5-en-2-one are described. These syntheses take advantage of a previously reported radical rearrangement (1,2-acyl migration). A remarkable iodide-mediated cleavage of a bicyclic system, followed by the introduction of the γ-chains via a mixed Kolbe electrolysis, are the key steps of these syntheses. This approach is general and could be applied for the preparation of all kinds of paraconic acids with excellent control of the stereochem.

ED Entered STN: 03 Jan 2003

IT 78-94-4, Methyl vinyl ketone
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

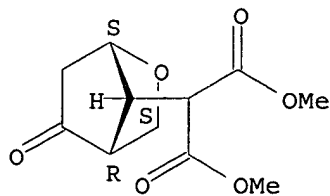


IT 152469-10-8P 501666-59-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
 (preparation of (-)-dihydropertusaric acid and formal synthesis of (±)-nephromopsinic, and (-)-phaseolinic acids)

RN 152469-10-8 HCAPLUS

CN Propanedioic acid, [(1R,4S,7R)-5-oxo-2-oxabicyclo[2.2.1]hept-7-yl]-, dimethyl ester, rel- (9CI) (CA INDEX NAME)

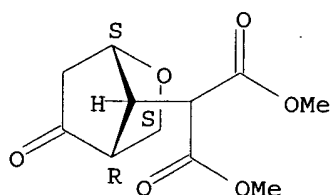
Relative stereochemistry.



RN 501666-59-7 HCAPLUS

CN Propanedioic acid, [(1S,4R,7S)-5-oxo-2-oxabicyclo[2.2.1]hept-7-yl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

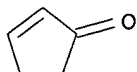


CC 26-6 (Biomolecules and Their Synthetic Analogs)
 Section cross-reference(s): 72
 IT **Asymmetric synthesis and induction**
 (of (-)-dihydropertusaric acid)
 IT **78-94-4**, Methyl vinyl ketone 109-52-4D, n-Pentanoic acid, derivs. 112-43-6, Undec-10-en-1-ol 127-19-5D, N,N-Dimethylacetamide, derivs. 638-53-9, Tridecanoic acid 72041-43-1 94482-75-4 95530-78-2, 7-Oxabicyclo[2.2.1]hept-5-en-2-one 501666-57-5
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (preparation of (-)-dihydropertusaric acid and formal synthesis of (+)-nephromopsinic, and (-)-phaseolinic acids)
 IT 39115-08-7P **152469-10-8P** 208587-00-2P 214531-60-9P 214531-61-0P 214531-62-1P 214531-63-2P 214531-64-3P 501666-52-0P 501666-53-1P 501666-54-2P 501666-55-3P 501666-56-4P 501666-58-6P **501666-59-7P** 501666-60-0P 501666-61-1P 501669-34-7P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
 (preparation of (-)-dihydropertusaric acid and formal synthesis of (+)-nephromopsinic, and (-)-phaseolinic acids)
 REFERENCE COUNT: 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

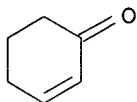
L93 ANSWER 12 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2003:3194 HCAPLUS
 DOCUMENT NUMBER: 138:353501
 TITLE: Enantioselective Michael addition and Henry reaction catalyzed by a new heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol
 AUTHOR(S): Rajasekhar, Ch V.; Maheswaran, H.
 CORPORATE SOURCE: Indian Institute of Chemical Technology, Hyderabad, 500 007, India
 SOURCE: Indian Journal of Chemistry, Section A: Inorganic, Bio-inorganic, Physical, Theoretical & Analytical Chemistry (2002), 41A(12), 2503-2506
 CODEN: ICACEC; ISSN: 0376-4710
 PUBLISHER: National Institute of Science Communication
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 138:353501

AB A heterobimetallic catalyst obtained by the reaction of LiAlH₄ with (+)-2,3-O-isopropylidene threitol promotes asym. Michael reaction (between malonic esters, and thiophenols to cyclic enones) as well as Henry reaction (between aliphatic and aromatic aldehydes and nitromethane) with excellent yields albeit low enantiomeric excesses.

ED Entered STN: 03 Jan 2003
 IT 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexenone
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (enantioselective Michael addition of cycloenones with malonates
 or thiophenols and Henry reaction of aldehydes with
 nitromethane catalyzed by heterobimetallic aluminum-lithium
 complex derived from (+)-2,3-O-isopropylidene threitol)
 RN 930-30-3 HCAPLUS
 CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

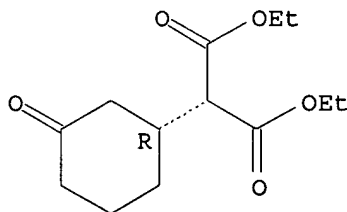


RN 930-68-7 HCAPLUS
 CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



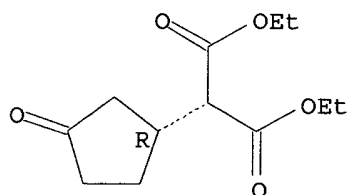
IT 164931-78-6P 194095-90-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (enantioselective Michael addition of cycloenones with malonates
 or thiophenols and Henry reaction of aldehydes with
 nitromethane catalyzed by heterobimetallic aluminum-lithium
 complex derived from (+)-2,3-O-isopropylidene threitol)
 RN 164931-78-6 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 194095-90-4 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, diethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 67

IT **Alkylation**

(Henry, nitroaldol; enantioselective **Michael** addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol)

IT **Asymmetric synthesis and induction**

(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol)

IT **Michael reaction**

(stereoselective; enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol)

IT 100-52-7, Benzaldehyde, reactions 104-53-0, 3-Phenylpropanal
104-87-0, p-Methylbenzaldehyde 105-53-3, Ethyl malonate
106-54-7, p-Chlorothiophenol 123-38-6, Propanal, reactions
930-30-3, 2-Cyclopentenone 930-68-7,
2-Cyclohexenone

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol)

IT 64924-10-3P 141434-97-1P 149495-00-1P **164931-78-6P**
194095-90-4P 259811-41-1P 518328-48-8P 518328-49-9P

RL: SPN (Synthetic preparation); **PREP (Preparation)**

(enantioselective Michael addition of cycloenones with malonates or thiophenols and Henry reaction of aldehydes with nitromethane catalyzed by heterobimetallic aluminum-lithium complex derived from (+)-2,3-O-isopropylidene threitol)

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 13 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:863839 HCAPLUS

DOCUMENT NUMBER: 139:85391

TITLE: Product subclass 16: silyl enol ethers

AUTHOR(S): Kobayashi, S.; Manabe, K.; Ishitani, H.;
Matsuo, J.-I.

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Hongo, Bunkyo-ku,
Tokyo, 113-0033, Japan

SOURCE: Science of Synthesis (2002), 4,

317-369

CODEN: SSCYJ9

PUBLISHER:

Georg Thieme Verlag

DOCUMENT TYPE:

Journal; General Review

LANGUAGE:

English

AB A review of preparation and reactions of silyl enol ethers. Covered reactions include addition, alkylation, Mukaiyama reaction, aldol condensation, cycloaddn., Mannich reaction, Diels-Alder reaction, amination, Ireland-Claisen rearrangement, hydroxylation, and silylation.

ED Entered STN: 14 Nov 2002

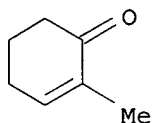
IT 1121-18-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(addition of furan and bis(trimethylsilane) amine; preparation of silyl enol ethers via reductive silylation of α,β -unsatd. carbonyl compound)

RN 1121-18-2 HCAPLUS

CN 2-Cyclohexen-1-one, 2-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



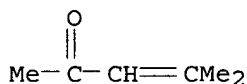
IT 141-79-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of silyl enol ethers via hydrosilylation of α,β -unsatd. carbonyl compound)

RN 141-79-7 HCAPLUS

CN 3-Penten-2-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



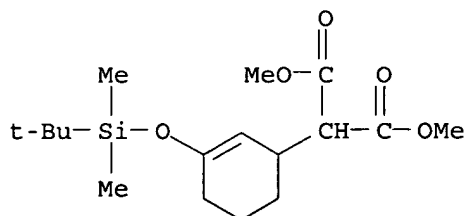
IT 152094-29-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of silyl enol ethers via reductive silylation of α,β -unsatd. carbonyl compound)

RN 152094-29-6 HCAPLUS

CN Propanedioic acid, [3-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]-2-cyclohexen-1-yl]-, dimethyl ester (9CI) (CA INDEX NAME)



CC 29-0 (Organometallic and Organometalloidal Compounds)

IT **Asymmetric synthesis and induction**
(asym. aldol reaction of chiral silyl enol ether with achiral benzaldehyde)

IT **1121-18-2**
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(addition of furan and bis(trimethylsilane) amine; preparation of silyl enol ethers via reductive silylation of α,β -unsatd. carbonyl compound)

IT **141-79-7** 18707-60-3
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(preparation of silyl enol ethers via hydrosilylation of α,β -unsatd. carbonyl compound)

IT 62790-93-6P 78905-92-7P 105229-94-5P 106251-78-9P
108612-95-9P 138593-34-7P 146273-75-8P **152094-29-6P**
160915-46-8P 177658-19-4DP, polymer-bound 441011-27-4P
556813-33-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of silyl enol ethers via reductive silylation of α,β -unsatd. carbonyl compound)

REFERENCE COUNT: 418 THERE ARE 418 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 14 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:863063 HCAPLUS

DOCUMENT NUMBER: 138:89950

TITLE: Enantioselective Total Synthesis of
(-)-Strychnine Using the Catalytic Asymmetric
Michael Reaction and Tandem Cyclization

AUTHOR(S): Ohshima, Takashi; Xu, Youjun; Takita, Ryo;
Shimizu, Satoshi; Zhong, Dafang; Shibasaki,
Masakatsu

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
University of Tokyo, Tokyo, 113-0033, Japan

SOURCE: Journal of the American Chemical Society (**2002**), 124(49), 14546-14547
CODEN: JACSAT; ISSN: 0002-7863

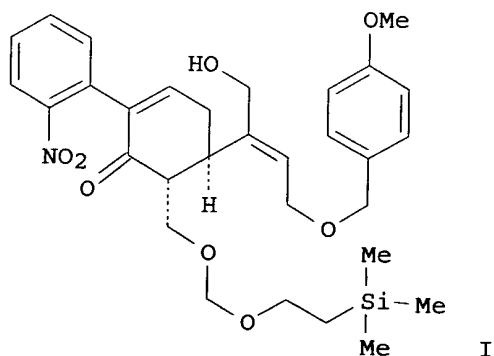
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:89950

GI



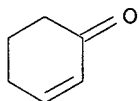
AB The enantioselective total synthesis of (-)-strychnine was accomplished through the use of the highly practical catalytic asym. Michael reaction of 2-cyclohexen-1-one with di-Me malonate (0.1 mol % of (R)-ALB, more than kilogram scale, without chromatog., 91% yield and >99% ee) as well as a tandem cyclization of (nitrophenyl)propenylcyclohexenone I that simultaneously constructed B- and D-rings (>77% yield). Moreover, newly developed reaction conditions for thionium ion cyclization, NaBH₃CN reduction of the imine moiety in the presence of Lewis acid to prevent ring opening reaction, and chemoselective reduction of the thioether (desulfurization) in the presence of exocyclic olefin were pivotal to complete the synthesis. The described chemical paves the way for the synthesis of more advanced Strychnos alkaloids.

ED Entered STN: 14 Nov 2002

IT 930-68-7, 2-Cyclohexen-1-one
RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

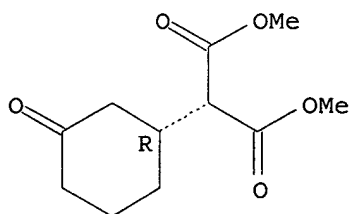


IT 164931-77-5P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 31-4 (Alkaloids)

IT **Asymmetric synthesis and induction**
(asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

IT **Michael reaction**
Michael reaction catalysts
(stereoselective; asym. total synthesis of (-)-strychnine via catalytic asym. Michael reaction and tandem cyclization)

IT 108-59-8, Dimethyl malonate 126-39-6, 2-Ethyl-2-methyl-1,3-

dioxolane 141-82-2, Malonic acid, reactions 930-68-7,
2-Cyclohexen-1-one 13154-24-0 17341-93-4, 2,2,2-
Trichloroethoxycarbonyl chloride 76513-69-4 80522-42-5,
Triisopropylsilyl triflate 122807-21-0 191731-32-5
482351-25-7

RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. total synthesis of (-)-strychnine via catalytic asym.
Michael reaction and tandem cyclization)

IT 509-40-0P 71366-23-9P 164931-77-5P 482351-05-3P
482351-06-4P 482351-07-5P 482351-08-6P 482351-09-7P
482351-10-0P 482351-11-1P 482351-12-2P 482351-13-3P
482351-14-4P 482351-15-5P 482351-16-6P 482351-18-8P
482351-19-9P 482351-20-2P 482351-21-3P 482351-22-4P
482351-26-8P 482351-27-9P 482351-28-0P 482351-29-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(asym. total synthesis of (-)-strychnine via catalytic asym.
Michael reaction and tandem cyclization)

REFERENCE COUNT: 31 THERE ARE 31 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 15 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:456602 HCAPLUS

DOCUMENT NUMBER: 138:4183

TITLE: Highly enantioselective catalytic Michael
reaction of α -substituted malonates
using La-linked-BINOL complex in the presence
of HFIP (1,1,1,3,3,3-hexafluoroisopropanol)
AUTHOR(S): Takita, Ryo; Ohshima, Takashi; Shibasaki,
Masakatsu

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Tokyo, 113-0033,
Japan

SOURCE: Tetrahedron Letters (2002), 43(26),
4661-4665

CODEN: TELEAY; ISSN: 0040-4039

PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 138:4183

AB A catalytic asym. Michael reaction of α -substituted
malonates with broad generality was developed using the
La-linked-BINOL complex. To enhance the reactivity of unreactive
 α -substituted malonates, the effects of concentration and additives
were examined; 1.0 M was the best concentration and HFIP
(1,1,1,3,3,3-hexafluoroisopropanol) accelerated the reaction
efficiently. Under the optimized conditions, the catalytic asym.
Michael reaction of a variety of α -substituted malonates
proceeded successfully in high yield (up to 93%) and excellent
enantiomeric excess (up to 99% ee). The addition of HFIP was also
effective for the reaction of nonsubstituted malonates. In this
case, 5 mol% of the La-linked-BINOL complex was sufficient for
completion of the reaction in approx. 24 h. Moreover, several
Michael adducts were readily converted to the bicyclic compds.

ED Entered STN: 18 Jun 2002

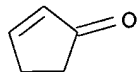
IT 930-30-3, 2-Cyclopentenone 930-68-7,
2-Cyclohexenone 1121-66-0, 2-Cycloheptenone

RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael reaction of malonates with

cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)

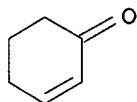
RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



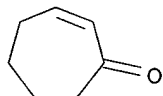
RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1121-66-0 HCAPLUS

CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



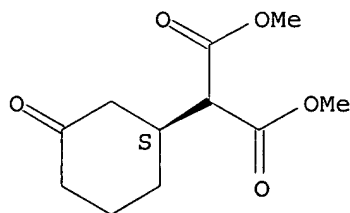
IT 154194-50-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael reaction of malonates with
cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)

RN 154194-50-0 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



CC 21-2 (General Organic Chemistry)

IT **Asymmetric synthesis and induction**

(enantioselective Michael reaction of malonates with
cycloalkenones using La-linked-BINOL complex
catalyst/hexafluoroisopropanol accelerator systems)

IT **Michael reaction**

Michael reaction catalysts

(stereoselective; enantioselective Michael reaction of

malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

IT 108-59-8, Dimethyl malonate 930-30-3, 2-Cyclopentenone 930-68-7, 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone 15014-25-2, Dibenzyl malonate 173541-54-3 173979-06-1 476437-46-4 476437-50-0 476437-52-2 476437-54-4 476437-55-5

RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael reaction of malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

IT 154194-47-5P 154194-49-7P 154194-50-0P 476437-56-6P 476437-58-8P 476437-59-9P 476437-61-3P 476437-65-7P 476437-67-9P 476437-71-5P

RL: SPN (Synthetic preparation); PREP (Preparation)
(enantioselective Michael reaction of malonates with cycloalkenones using La-linked-BINOL complex catalyst/hexafluoroisopropanol accelerator systems)

REFERENCE COUNT: 24 THERE ARE 24 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 16 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:169599 HCAPLUS

DOCUMENT NUMBER: 136:240696

TITLE: Preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asymmetric Michael addition reaction

INVENTOR(S): Shibazaki, Masakatsu; Oshima, Takashi; Matsunaga, Shigeki

PATENT ASSIGNEE(S): Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
CODEN: JKXXAF

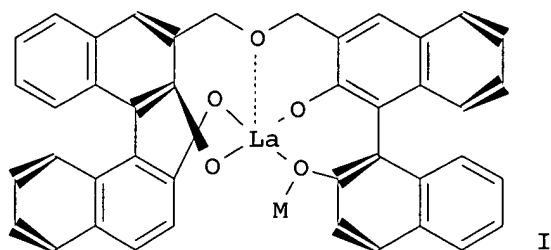
DOCUMENT TYPE: Patent

LANGUAGE: Japanese

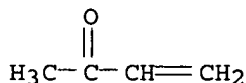
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

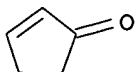
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2002069076	A2	20020308	JP 2000-262411	2000 0831
TW 552265	B	20030911	TW 2000-89118379	2000 0905
PRIORITY APPLN. INFO.: JP 2000-262411 A 2000 0831				
OTHER SOURCE(S): CASREACT 136:240696				



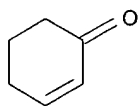
- AB The bis[[(1R,1'R)-2,2'-dihydroxy-1,1'-binaphthyl-3-yl]methyl] ether-lanthanum complexes (I; M = H, monovalent metal atom) and an acid composition containing I are prepared. These complexes I catalyze asym. Michael addition reaction of β -dicarbonyl compds. with cyclic or noncyclic enones. They are very stable even in air and can be stored for a long period of time and reused. Thus, 7.5 mL of 0.2M $\text{La}(\text{O}-i\text{-Pr})_3/\text{THF}$ (1.5 mmol) was added to a solution of 1.01 g bis[[(1R,1'R)-2,2'-Dihydroxy-1,1'-binaphthyl-3-yl]methyl] ether (containing 7.4 weight/weight% Et_2O and hexane) in 10 mL THF and stirred at room temperature for 5 h to give 1.13 g I (M = H). I (M = H) (45.1 mg) was added to 1.5 mL 1,2-dimethoxyethane at -78° in an acetone-dry ice bath and stirred for 5 min, followed by adding 58 μL 2-cyclohexen-1-one (0.60 mmol) and 150 μL dibenzyl malonate (0.60 mmol), and the resulting mixture was stirred at -78° in the acetone-dry ice bath and at 4° for 85 h after removing the bath to give 98% (R)-3-[bis(benzyloxycarbonyl)methyl]cyclohexanone (>99% ee).
- ED Entered STN: 08 Mar 2002
- IT 78-94-4, Methyl vinyl ketone, reactions 930-30-3, 2-Cyclopentenone 930-68-7, 2-Cyclohexen-1-one 1121-66-0, 2-Cycloheptenone
- RL: RCT (Reactant); RACT (Reactant or reagent)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)
- RN 78-94-4 HCAPLUS
- CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



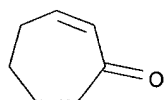
- RN 930-30-3 HCAPLUS
- CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



- RN 930-68-7 HCAPLUS
- CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

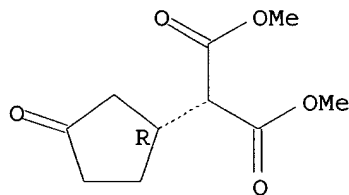


RN 1121-66-0 HCAPLUS
 CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



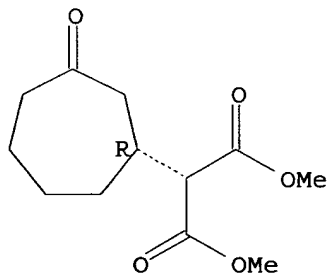
IT 287493-81-6P, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclopentanone 287493-82-7P, (R)-(+)-3-[1,1-Bis(methoxycarbonyl)methyl]cycloheptanone 403620-79-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
 (preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)
 RN 287493-81-6 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocyclopentyl]-, dimethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



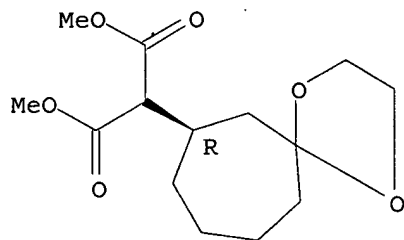
RN 287493-82-7 HCAPLUS
 CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 403620-79-1 HCAPLUS
 CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.6]undec-7-yl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



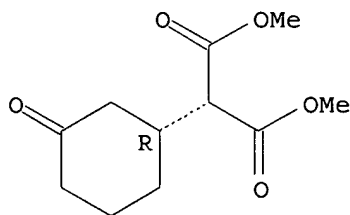
IT 164931-77-5P, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclohexanone 287493-83-8P, (R)-(-)-3-[1,1-Bis(methoxycarbonyl)methyl]cyclooctanone 287493-86-1P, (R)-(-)-2-(Methoxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid methyl ester 403620-77-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)

RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

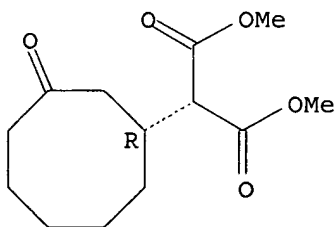
Absolute stereochemistry. Rotation (+).



RN 287493-83-8 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclooctyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

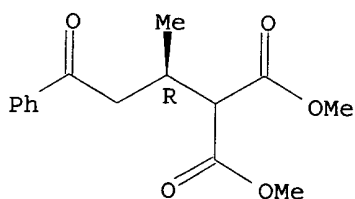
Absolute stereochemistry. Rotation (-).



RN 287493-86-1 HCAPLUS

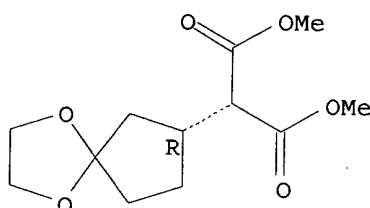
CN Propanedioic acid, [(1R)-1-methyl-3-oxo-3-phenylpropyl]-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 403620-77-9 HCAPLUS
 CN Propanedioic acid, (7R)-1,4-dioxaspiro[4.4]non-7-yl-, dimethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



- IC ICM C07F005-00
 ICS B01J031-22; C07B053-00; C07C043-178; C07C067-333;
 C07C069-716; C07C069-757; C07D317-60; C07D317-72; C07B061-00;
 C07M007-00
- CC 78-7 (Inorganic Chemicals and Reactions)
 Section cross-reference(s): 24, 25, 28
- IT **Asymmetric synthesis and induction**
 (preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)
- IT **Michael reaction**
 (stereoselective; preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)
- IT 78-94-4, Methyl vinyl ketone, reactions 108-59-8,
 Dimethyl malonate 126-39-6, 2-Ethyl-2-methyl-1,3-dioxolane
 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexen-1-one 1121-66-0, 2-Cycloheptenone
 1195-60-4, 2-Cyclononenone 1655-07-8, Ethyl 2-oxocyclohexanecarboxylate 1728-25-2, 2-Cyclooctenone
 15014-25-2, Dibenzyl malonate 19446-52-7, Lanthanum isopropoxide
 35845-66-0 82794-36-3, Dibenzyl methylmalonate
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)
- IT 185760-71-8P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cyclopentanone 185760-72-9P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cycloheptanone 287493-81-6P, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclopentanone 287493-82-7P, (R)-(+)-3-[1,1-Bis(methoxycarbonyl)methyl]cycloheptanone 403620-79-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)

IT 69881-57-8P, (R)-(+)-2-Oxo-1-(3-oxobutyl)cyclohexane-1-carboxylic acid ethyl ester 164931-75-3P, (R)-(+)-3-[Bis(benzyloxycarbonyl)methyl]cyclohexanone 164931-76-4P, (R)-(+)-3-[1,1-Bis(benzyloxycarbonyl)ethyl]cyclohexanone 164931-77-5P, (R)-(+)-3-[Bis(methoxycarbonyl)methyl]cyclohexanone 287493-83-8P, (R)-(-)-3-[1,1-Bis(methoxycarbonyl)methyl]cyclooctanone 287493-84-9P, (R)-(-)-3-[1,1-Bis(benzyloxycarbonyl)methyl]cyclononanone 287493-85-0P, (R)-(-)-2-(Benzyloxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid benzyl ester 287493-86-1P, (R)-(-)-2-(Methoxycarbonyl)-3-methyl-5-oxo-5-phenylpentanoic acid methyl ester 403620-76-8P 403620-77-9P 403620-78-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of lanthanum-linked bis(BINOL) complexes as catalysts for asym. Michael addition reactions of cyclic or noncyclic enones with β -dicarbonyl compds.)

L93 ANSWER 17 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2002:153736 HCAPLUS

DOCUMENT NUMBER: 137:169294

TITLE: Efficient Mukaiyama aldol reaction by silver(I) carboxylate-bis(phosphine) catalysts
AUTHOR(S): Ohkouchi, Munetaka; Masui, Dai; Yamaguchi, Motowo; Yamagishi, Takamichi

CORPORATE SOURCE: Department of Applied Chemistry, Graduate School of Engineering, Tokyo Metropolitan University, Hachioji-shi, 192-0397, Japan

SOURCE: Nippon Kagaku Kaishi (2002), (2), 223-229

CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER: Nippon Kagakkai

DOCUMENT TYPE: Journal

LANGUAGE: Japanese

OTHER SOURCE(S): CASREACT 137:169294

AB Silver(I) carboxylate-BINAP complex, water tolerant and air-stable, is a highly efficient catalyst for Mukaiyama aldol reaction using silyl enol ethers or ketene silyl acetals as nucleophiles. The Mukaiyama aldol reaction of aldehydes or keto esters in DMF afforded aldol products quant. in a short reaction time by this silver(I) carboxylate-BINAP catalyst. Using ketene silyl acetals, aliphatic ketones also gave the aldol products in high yields, however, with aromatic ketones both aldol reaction and silyl transfer reaction were observed. The silver(I) carboxylate-BINAP catalyst acts as a good catalyst for Mukaiyama Michael addition of α,β -unsatd. ketones. The catalyst strongly activates nucleophiles to cause the aldol reaction easily.

ED Entered STN: 28 Feb 2002

IT 930-68-7, 2-Cyclohexenone 74311-56-1,

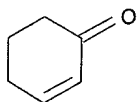
(S)-(R)-BPPFA

RL: RCT (Reactant); RACT (Reactant or reagent)

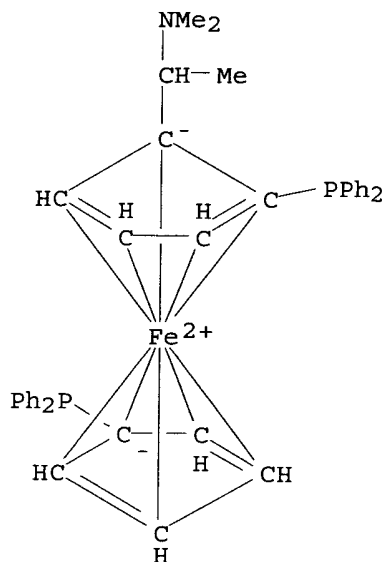
(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) catalysts)

RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 74311-56-1 HCAPLUS
 CN Ferrocene, 1-[(1R)-1-(dimethylamino)ethyl]-1',2-bis(diphenylphosphino)-, (2S)- (9CI) (CA INDEX NAME)



CC 25-18 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 78

IT **Asymmetric synthesis and induction**

Michael reaction

Michael reaction catalysts

(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) catalysts)

IT 66-77-3, 1-Naphthaldehyde 66-99-9, 2-Naphthaldehyde 67-64-1, Acetone, reactions 98-86-2, Acetophenone, reactions 100-06-1, p-Methoxyacetophenone 100-19-6, p-Nitroacetophenone 100-52-7, Benzaldehyde, reactions 108-94-1, Cyclohexanone, reactions 110-62-3, Butyraldehyde 134-81-6, Benzil 563-63-3, Silver(I) acetate 600-22-6, Methyl pyruvate 614-47-1 709-63-7, p-Trifluoromethylacetophenone 930-68-7, 2-Cyclohexenone 1896-62-4 6651-36-1 6737-42-4, DPPP 7688-25-7, DPPB 13735-81-4, Acetophenone trimethylsilyl enol ether 14371-10-9, trans-Cinnamaldehyde 15206-55-0, Methyl phenyloxoacetate 31469-15-5 31469-16-6 37002-48-5, (S,S)-DIOP 66323-99-7 **74311-56-1**, (S)-(R)-BPPFA 76189-56-5, (S)-BINAP 100165-88-6, (S)-Tol-BINAP

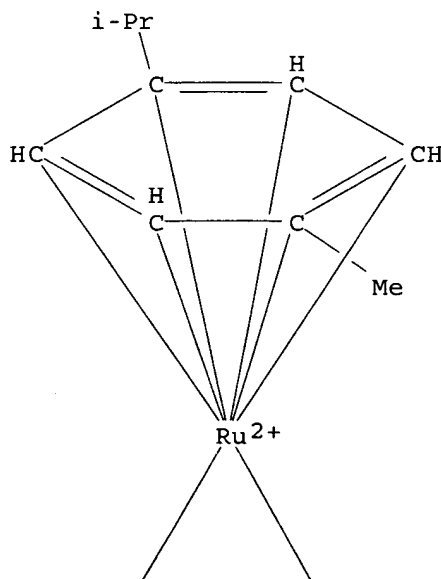
RL: RCT (Reactant); **RACT (Reactant or reagent)**

(efficient Mukaiyama aldol reaction or Mukaiyama Michael addition by silver(I) carboxylate-bis(phosphine) catalysts)

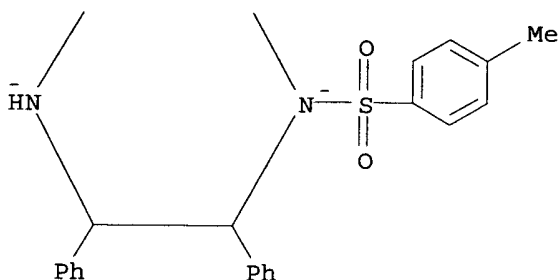
L93 ANSWER 18 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 2001:420228 HCAPLUS

DOCUMENT NUMBER: 135:241689
TITLE: Catalytic asymmetric Michael reactions using a chiral rhodium complex
AUTHOR(S): Suzuki, T.; Torii, T.
CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Tokyo, Bunkyo-ku,
Hongo, 113-0033, Japan
✓ SOURCE: Tetrahedron: Asymmetry (2001),
12(7), 1077-1081
CODEN: TASYE3; ISSN: 0957-4166
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 135:241689
AB Catalytic asym. Michael reaction of β -keto esters and Me
vinyl ketone was achieved using a chiral diamine-based Rh complex
to give the Michael adducts in up to 75% e.e.
ED Entered STN: 11 Jun 2001
IT 195516-84-8
RL: CAT (Catalyst use); USES (Uses)
(asym. Michael reaction catalyzed by chiral rhodium complex)
RN 195516-84-8 HCAPLUS
CN Ruthenium, [N-[(1R,2R)-2-amino-1,2-diphenylethyl]-4-
methylbenzenesulfonamido(2-)- κ N][(1,2,3,4,5,6- η)-1-
methyl-4-(1-methylethyl)benzene]- (9CI) (CA INDEX NAME)

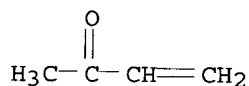
PAGE 1-A



PAGE 2-A

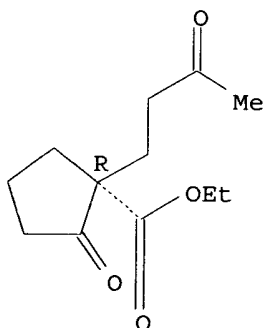


IT 78-94-4, Methyl vinyl ketone, reactions
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (asym. Michael reaction catalyzed by chiral rhodium complex)
 RN 78-94-4 HCAPLUS
 CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



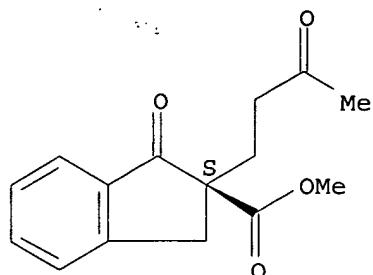
IT 58623-79-3P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (asym. Michael reaction catalyzed by chiral rhodium complex)
 RN 58623-79-3 HCAPLUS
 CN Cyclopentanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester,
 (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



IT 58623-84-0P 69881-57-8P 78044-62-9P
 360795-53-5P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. Michael reaction catalyzed by chiral rhodium complex)
 RN 58623-84-0 HCAPLUS
 CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-,
 methyl ester, (2S)- (9CI) (CA INDEX NAME)

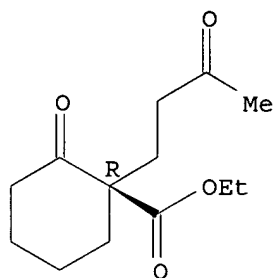
Absolute stereochemistry. Rotation (-).



RN 69881-57-8 HCAPLUS

CN Cyclohexanecarboxylic acid, 2-oxo-1-(3-oxobutyl)-, ethyl ester,
(1R)- (9CI) (CA INDEX NAME)

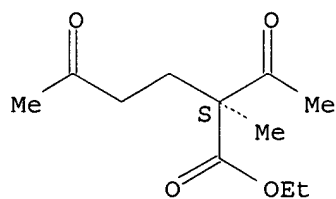
Absolute stereochemistry. Rotation (+).



RN 78044-62-9 HCAPLUS

CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI)
(CA INDEX NAME)

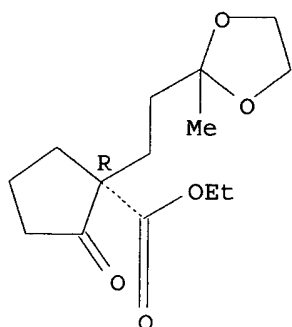
Absolute stereochemistry. Rotation (-).



RN 360795-53-5 HCAPLUS

CN Cyclopentanecarboxylic acid, 1-[2-(2-methyl-1,3-dioxolan-2-yl)ethyl]-2-oxo-, ethyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 21-2 (General Organic Chemistry)

IT **Michael reaction**

Michael reaction catalysts

(stereoselective; asym. Michael reaction catalyzed by chiral rhodium complex)

IT 12354-84-6 12354-85-7 52462-29-0 78615-08-4 144222-34-4
195516-84-8 360795-52-4

RL: CAT (Catalyst use); USES (Uses)

(asym. Michael reaction catalyzed by chiral rhodium complex)

IT **78-94-4**, Methyl vinyl ketone, reactions 609-14-3

611-10-9 1655-07-8 22955-77-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. Michael reaction catalyzed by chiral rhodium complex)

IT **58623-79-3P**

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(asym. Michael reaction catalyzed by chiral rhodium complex)

IT **58623-84-0P 69881-57-8P 78044-62-9P**
360795-53-5P

RL: SPN (Synthetic preparation); PREP (Preparation)

(asym. Michael reaction catalyzed by chiral rhodium complex)

REFERENCE COUNT: 48 THERE ARE 48 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 19 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2001:12419 HCAPLUS

DOCUMENT NUMBER: 134:86044

TITLE: Preparation of chiral 2-amino-2'-
diphenylphosphino-1,1'-binaphthyl derivatives
as metal catalyst ligands

INVENTOR(S): Zhang, Xumu

PATENT ASSIGNEE(S): The Penn State Research Foundation, USA

SOURCE: PCT Int. Appl., 93 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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WO 2001000581	A1	20010104	WO 2000-US17903	2000

0629

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W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN,
CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM,
HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ,
PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT,
TZ, UA, UG, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD,
RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE,
CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL,
PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE,
SN, TD, TG

US 6380392

B1

20020430

US 2000-607005

2000

0629

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PRIORITY APPLN. INFO.:

US 1999-141795P

P

1999

0630

<--

OTHER SOURCE(S):

CASREACT 134:86044; MARPAT 134:86044

AB Title ligands are bidentate, tridentate, tetradentate, or
pentadentate and include P-P, P-N, N-N, mixed P-N, Schiff base or
carbene sites. Transition metal complexes with these ligands are
effective catalysts for asym. reactions. Thus, Et₂Zn addition to
2-cyclohexenone in the presence of (S)-2-(2-
pyridinylcarbonylamino)-2'-diphenylphosphino-1,1'-binaphthyl
complex with Cu gave (S)-3-ethylcyclohexanone of 92% ee with 98%
conversion.

ED Entered STN: 05 Jan 2001

IT 316831-08-0P

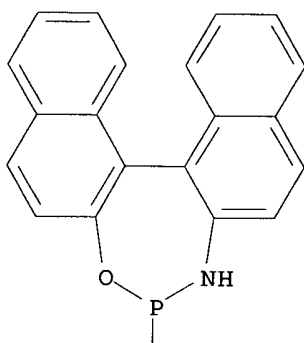
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)

(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl
derivs. as metal catalyst ligands)

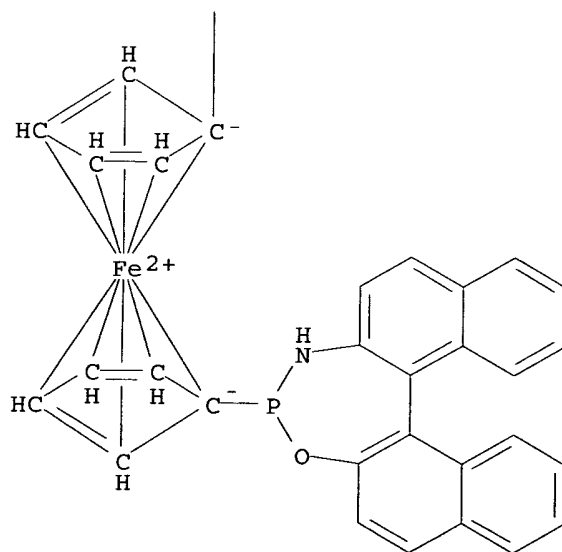
RN 316831-08-0 HCAPLUS

CN Ferrocene, 1,1'-bis(dinaphth[2,1-d:1',2'-f][1,3,2]oxazaphosphepin-
4(5H)-yl)- (9CI) (CA INDEX NAME)

PAGE 1-A

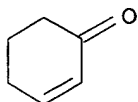


PAGE 2-A



IT 930-68-7, 2-Cyclohexenone 1821-29-0,
 (E)-5-Methyl-3-hexen-2-one
 RL: RCT (Reactant); **RACT** (Reactant or reagent)
 (preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl
 derivs. as metal catalyst ligands)
 RN 930-68-7 HCAPLUS

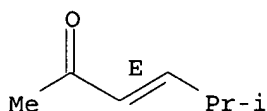
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



RN 1821-29-0 HCAPLUS

CN 3-Hexen-2-one, 5-methyl-, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IC ICM C07D213-81

ICS C07D237-20; C07D307-52; C07D333-38; C07F009-53

CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 21

IT **Asymmetric synthesis and induction**

(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)

IT **Michael reaction**

(stereoselective, catalysts; preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)

IT	259260-34-9P	259260-35-0P	316811-92-4P	316811-94-6P
	316811-96-8P	316811-98-0P	316812-00-7P	316812-03-0P
	316812-05-2P	316812-07-4P	316812-09-6P	316812-11-0P
	316812-13-2P	316812-15-4P	316812-17-6P	316812-19-8P
	316812-21-2P	316812-23-4P	316812-25-6P	316812-27-8P
	316812-29-0P	316812-31-4P	316812-33-6P	316812-35-8P
	316812-37-0P	316812-39-2P	316812-41-6P	316812-43-8P
	316812-45-0P	316812-47-2P	316812-49-4P	316812-51-8P
	316812-53-0P	316812-56-3P	316812-59-6P	316812-61-0P
	316812-63-2P	316812-65-4P	316812-67-6P	316812-69-8P
	316812-71-2P	316812-72-3P	316812-73-4P	316812-74-5P
	316812-75-6P	316831-08-0P	317330-09-9P	317330-10-2P
	317330-11-3P	317330-12-4P	317330-13-5P	317330-14-6P
	317330-15-7P	317330-16-8P	317330-17-9P	317330-18-0P
	317330-19-1P	317330-79-3P		

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl derivs. as metal catalyst ligands)

IT 98-98-6, 2-Pyridinecarboxylic acid 100-42-5, Styrene, reactions
 135-19-3, 2-Naphthol, reactions 602-09-5, 1,1'-Bi-2-naphthol
 614-47-1, trans-1,3-Diphenyl-2-propen-1-one 623-73-4, Ethyl
 diazoacetate 930-68-7, 2-Cyclohexenone 934-60-1,
 2-Carboxy-6-methylpyridine 1013-88-3, Iminodiphenylmethane
 1121-60-4, 2-Pyridinecarboxaldehyde 1122-72-1,
 6-Methyl-2-Pyridinecarboxaldehyde 1195-59-1,
 2,6-Pyridinedimethanol 1821-29-0, (E)-5-Methyl-3-hexen-2-
 one 1896-62-4, (E)-4-Phenyl-3-buten-2-one 3739-94-4,

2,6-Pyridinedicarbonyl chloride 4559-70-0, Diphenylphosphine
oxide 22252-15-9, (E)-3-(4-Methoxyphenyl)-1-phenyl-2-propen-1-
one 22252-16-0, (E)-3-(4-Chlorophenyl)-1-phenyl-2-propen-1-one
22966-19-4, (E)-1-(4-Methoxyphenyl)-3-phenyl-2-propen-1-one
22966-22-9, (E)-1-(4-Chlorophenyl)-3-phenyl-2-propen-1-one
37942-07-7, 3,5-Di-tert-butyl-2-hydroxybenzaldehyde

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(preparation of chiral 2-amino-2'-diphenylphosphino-1,1'-binaphthyl
derivs. as metal catalyst ligands)

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 20 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:845259 HCAPLUS

DOCUMENT NUMBER: 134:131299

TITLE: Immobilization of asymmetric multifunctional
catalysts on an insoluble polymer

AUTHOR(S): Matsunaga, Shigeki; Ohshima, Takashi;
Shibasaki, Masakatsu

CORPORATE SOURCE: Graduate School of Pharmaceutical Sciences,
The University of Tokyo, Tokyo, 113-0033,
Japan

SOURCE: Tetrahedron Letters (2000), 41(44),
8473-8478

PUBLISHER: CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Elsevier Science Ltd.

LANGUAGE: Journal

OTHER SOURCE(S): English

CASREACT 134:131299

AB A polymer-supported linked-BINOL was synthesized to immobilize
asym. catalysts with two BINOL units. The advantage of the
polymer-supported linked-BINOL over randomly polymer-supported
BINOL was confirmed by asym. Michael reaction. A novel
polymer-supported La-Zn-linked-BINOL complex afforded the Michael
adduct in good yield and moderate ee.

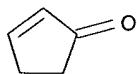
ED Entered STN: 05 Dec 2000

IT 930-30-3, 2-Cyclopentenone 930-68-7,
2-Cyclohexenone 1121-66-0, 2-Cycloheptenone

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction catalyzed by lanthanum
binaphthalenediol complex)

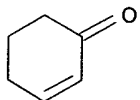
RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

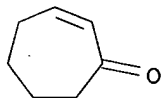


RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

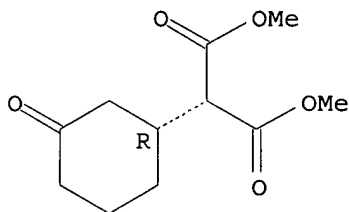


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



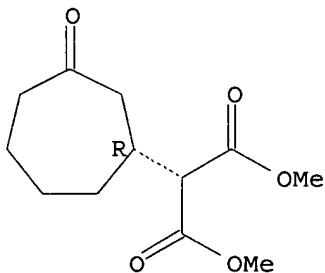
IT 164931-77-5P 287493-82-7P
RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reaction catalyzed by lanthanum
binaphthalenediol complex)
RN 164931-77-5 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



RN 287493-82-7 HCAPLUS
CN Propanedioic acid, [(1R)-3-oxocycloheptyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 25-24 (Benzene, Its Derivatives, and Condensed Benzenoid
Compounds)
Section cross-reference(s): 67, 78
IT **Asymmetric synthesis and induction**
(preparation of polymer-supported binaphthalenediol dimer as asym.
Michael catalyst)
IT **Michael reaction**
Michael reaction catalysts
(stereoselective; preparation of polymer-supported binaphthalenediol
dimer as asym. Michael catalyst)
IT 108-59-8, Dimethyl malonate 930-30-3, 2-Cyclopentenone

930-68-7, 2-Cyclohexenone 1121-66-0,
2-Cycloheptenone 15014-25-2, Dibenzyl malonate

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(asym. Michael reaction catalyzed by lanthanum
binaphthalenediol complex)

IT 164931-75-3P **164931-77-5P** 185760-71-8P 185760-72-9P
287493-82-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael reaction catalyzed by lanthanum
binaphthalenediol complex)

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 21 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 2000:145263 HCAPLUS

DOCUMENT NUMBER: 132:308474

TITLE: Cationic [2,6-Bis(2'-
oxazoliny)phenyl]palladium(II) Complexes:
Catalysts for the Asymmetric Michael Reaction
AUTHOR(S): Stark, Mark A.; Jones, Geraint; Richards,
Christopher J.

CORPORATE SOURCE: Department of Chemistry, Cardiff University,
Cardiff, CF10 3TB, UK

SOURCE: Organometallics (2000), 19(7),
1282-1291

CODEN: ORGND7; ISSN: 0276-7333

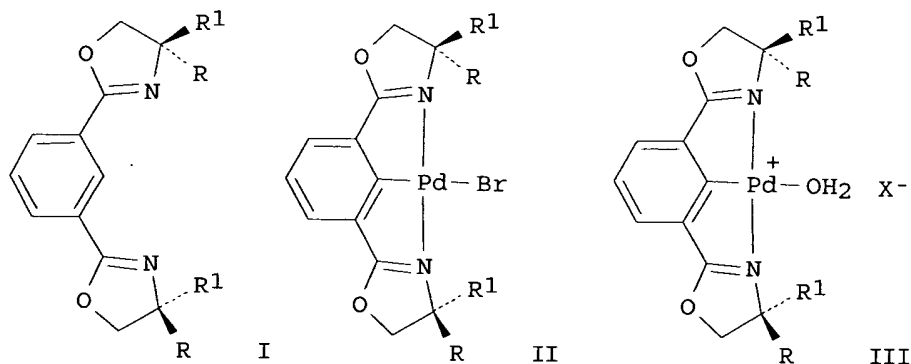
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 132:308474

GI



AB Reaction of 1,3-dicyanobenzene with β -amino alcs.

(S)-H₂NCHRCH₂OH (R = iPr, iBu, tBu, CH₂Cy, CH₂Ph) and

(R)-H₂NCHPhCH₂OH gave new 1,3-bis(2-oxazolin-2-yl)benzenes (I; R =
R₁ = Me; R = iPr, iBu, tBu, CH₂Cy, CH₂Ph, R₁ = H; R = H, R₁ = Ph)
(30-51%). These, together with 1,3-bis(4,4-dimethyl-2-oxazolin-2-
yl)benzene, were treated with LDA/TMEDA followed by the addition of
PdBr₂(1,5-COD) to give [2,6-bis(2-oxazolin-2-
yl)phenyl]palladium(II) bromide complexes (II; R = R₁ = Me; R =

iPr, iBu, tBu, CH₂Cy R₁ = H (Cy = cyclohexyl)) (21-41%). In two cases no complexes were obtained (with reactant I; R = H, R₁ = Ph; R = CH₂Ph, R₁ = H) due to ring opening of the oxazolines by LDA/TMEDA. Treatment of the Pd complexes II with AgBF₄, AgOTf, or AgSbF₆ in wet CH₂Cl₂ provided cationic [2,6-bis(2-oxazolin-2-yl)phenyl]palladium complexes (III; R, R₁ same as above, X⁻ = BF₄⁻, F₃CSO₃⁻, SbF₆⁻) (28-87%) containing H₂O coordinated to Pd, as established by an x-ray crystal structure anal. of (S,S)-[2,6-bis(4-isopropyl-2-oxazolin-2-yl)phenyl]aquaopalladium(II) trifluoromethanesulfonate (III; R = iPr, R₁ = H, X⁻ = F₃CSO₃⁻). All of the cationic complexes proved to be efficient catalysts for the Michael reaction between α-cyanocarboxylates and Me vinyl ketone and between acrylonitrile and activated Michael donors. Selectivities of up to 34% ee were obtained for the formation of (R)-Et 2-cyano-2-methyl-5-oxohexanoate.

ED Entered STN: 05 Mar 2000

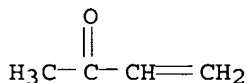
IT 78-94-4, 3-Buten-2-one, reactions

RL: RCT (Reactant); **RACT (Reactant or reagent)**

([bis(oxazolinyl)phenyl]palladium(II) cationic complex-catalyzed asym. Michael reaction of)

RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



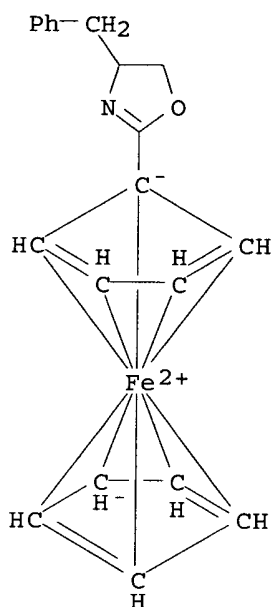
IT 162157-05-3, (S)-2-Ferrocenyl-4-benzyl-2-oxazoline

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(benzylic deprotonation followed by reaction with acid)

RN 162157-05-3 HCAPLUS

CN Ferrocene, [(4S)-4,5-dihydro-4-(phenylmethyl)-2-oxazolyl]- (9CI)
(CA INDEX NAME)



IT 196207-76-8P

RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)

RN 196207-76-8 HCAPLUS

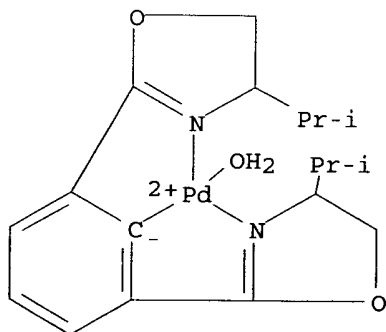
CN Palladium(1+), aqua [2,6-bis[(4S,4'S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 196207-75-7

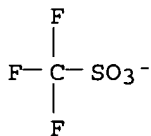
CMF C18 H25 N2 O3 Pd

CCI CCS



CM 2

CRN 37181-39-8
CMF C F3 O3 S



IT 196207-77-9P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation as catalyst for asym. Michael reaction and substitution reaction with nitriles)

RN 196207-77-9 HCAPLUS

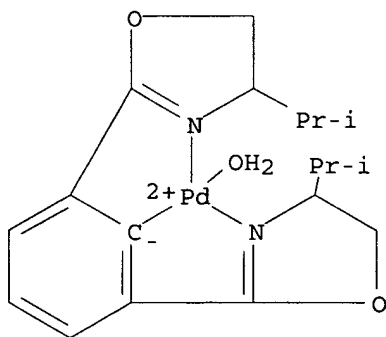
CN Palladium(1+), aqua[2,6-bis[(4S,4'S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 196207-75-7

CMF C18 H25 N2 O3 Pd

CCI CCS

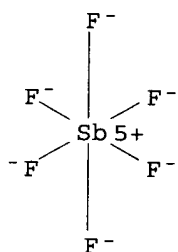


CM 2

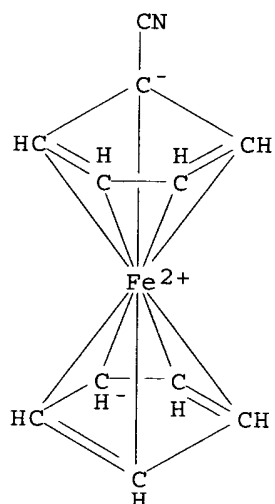
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CMF F6 Sb

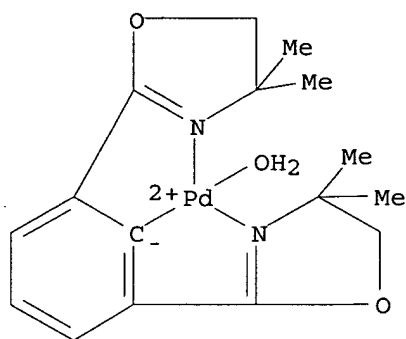
CCI CCS



IT 1273-84-3P, Ferrocenyl cyanide 196207-74-6P
 265127-72-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 1273-84-3 HCAPLUS
 CN Ferrocene, cyano- (9CI) (CA INDEX NAME)



RN 196207-74-6 HCAPLUS
 CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl-
 κN3)phenyl-κC]-, (SP-4-3)-, tetrafluoroborate(1-)
 (9CI) (CA INDEX NAME)
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 CRN 196207-73-5
 CMF C16 H21 N2 O3 Pd
 CCI CCS

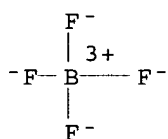


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



RN 265127-72-8 HCAPLUS

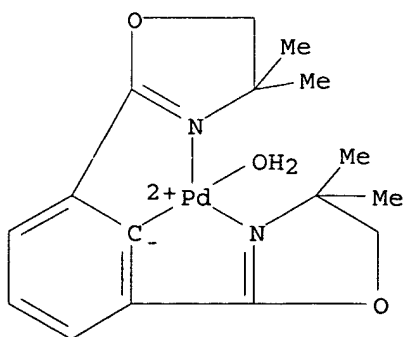
CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl- κ N3)phenyl- κ C]-, (SP-4-3)-, salt with trifluoromethanesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 196207-73-5

CMF C16 H21 N2 O3 Pd

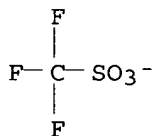
CCI CCS



CM 2

CRN 37181-39-8

CMF C F3 O3 S



IT 196207-80-4P 196207-82-6P 265127-73-9P

265127-74-0P 265127-76-2P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP
(Preparation); USES (Uses)(preparation of cationic [bis(oxazolinyl)phenyl]palladium(II)
complexes as catalysts for asym. Michael reaction)

RN 196207-80-4 HCAPLUS

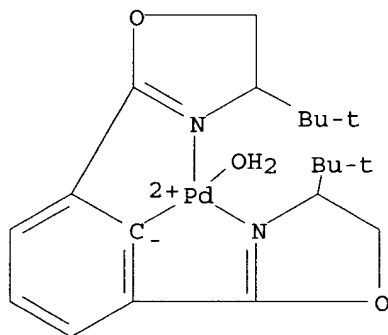
CN Palladium(1+), aqua[2,6-bis[(4S,5S)-4-(1,1-dimethylethyl)-4,5-
dihydro-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-,
(OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 196207-79-1

CMF C20 H29 N2 O3 Pd

CCI CCS

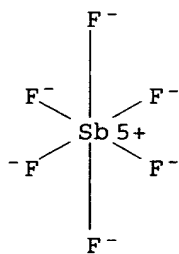


CM 2

CRN 17111-95-4

CMF F6 Sb

CCI CCS

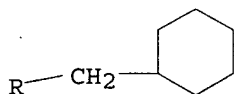
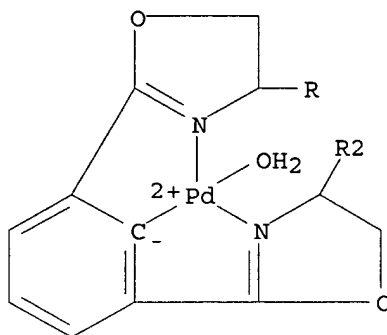


RN 196207-82-6 HCAPLUS
 CN Palladium(1+), aqua[2,6-bis[(4S)-4-(cyclohexylmethyl)-4,5-dihydro-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

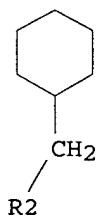
CM 1

CRN 196207-81-5
 CMF C26 H37 N2 O3 Pd
 CCI CCS

PAGE 1-A

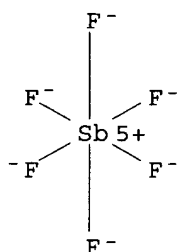


PAGE 2-A



CM 2

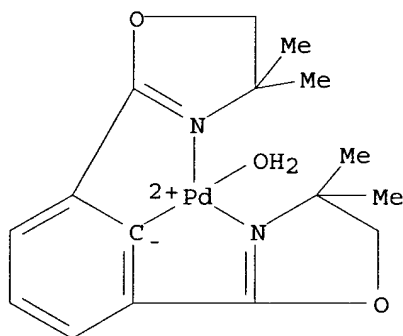
CRN 17111-95-4
 CMF F6 Sb
 CCI CCS



RN 265127-73-9 HCAPLUS
 CN Palladium(1+), aqua[2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl- κ N3)phenyl- κ C]-, (SP-4-3)-, (OC-6-11)-
 hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

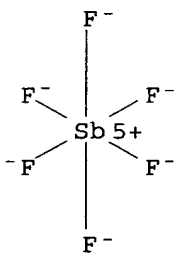
CM 1

CRN 196207-73-5
 CMF C16 H21 N2 O3 Pd
 CCI CCS



CM 2

CRN 17111-95-4
 CMF F6 Sb
 CCI CCS

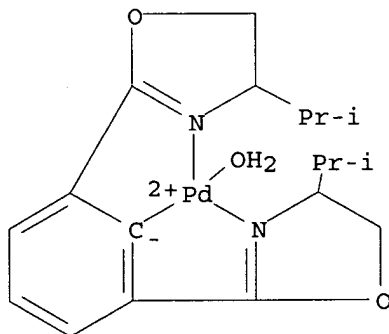


RN 265127-74-0 HCAPLUS
 CN Palladium(1+), aqua[2,6-bis[(4S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl- κ N3]phenyl- κ C]-, (SP-4-3)-,

tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

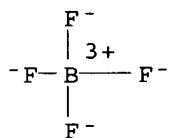
CM 1

CRN 196207-75-7
CMF C18 H25 N2 O3 Pd
CCI CCS



CM 2

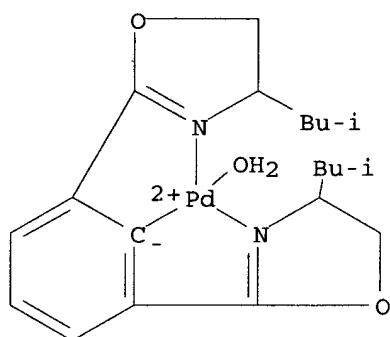
CRN 14874-70-5
CMF B F4
CCI CCS



RN 265127-76-2 HCAPLUS
CN Palladium(1+), aqua[2,6-bis[(4S)-4,5-dihydro-4-(2-methylpropyl)-2-oxazolyl-κN3]phenyl-κC]-, (SP-4-3)-, (OC-6-11)-hexafluoroantimonate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 265127-75-1
CMF C20 H29 N2 O3 Pd
CCI CCS

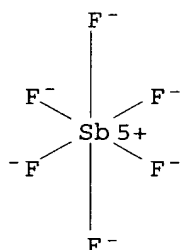


CM 2

CRN 17111-95-4

CMF F6 Sb

CCI CCS



IT 189632-52-8P 196207-70-2P 196207-71-3P

196207-72-4P 265127-67-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

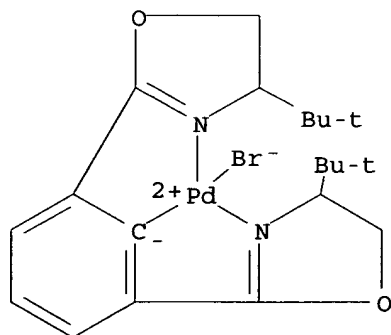
(preparation of cationic palladium bis(oxazolinyl)benzene aquo complexes from)

RN 189632-52-8 HCAPLUS

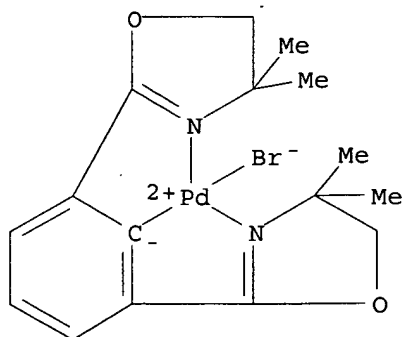
CN Palladium, [2,6-bis[(4S)-4-(1,1-dimethylethyl)-4,5-dihydro-2-

oxazolyl-κN3]phenyl-κC]bromo-, (SP-4-3) - (9CI) (CA

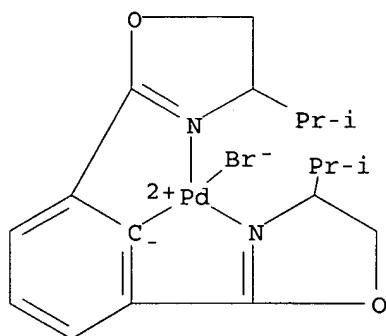
INDEX NAME)



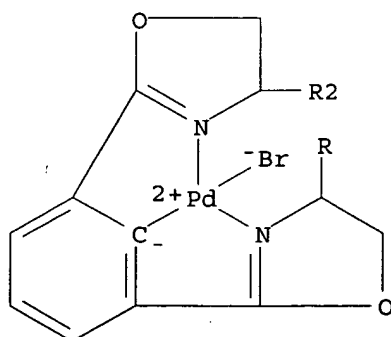
RN 196207-70-2 HCAPLUS
 CN Palladium, [2,6-bis(4,5-dihydro-4,4-dimethyl-2-oxazolyl- κ N3)phenyl- κ C]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



RN 196207-71-3 HCAPLUS
 CN Palladium, [2,6-bis[(4S)-4,5-dihydro-4-(1-methylethyl)-2-oxazolyl- κ N3]phenyl- κ C]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)

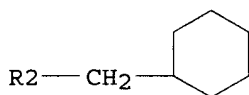
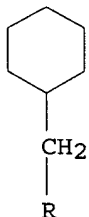


RN 196207-72-4 HCAPLUS
 CN Palladium, [2,6-bis[(4S)-4-(cyclohexylmethyl)-4,5-dihydro-2-oxazolyl- κ N3]phenyl- κ C]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)

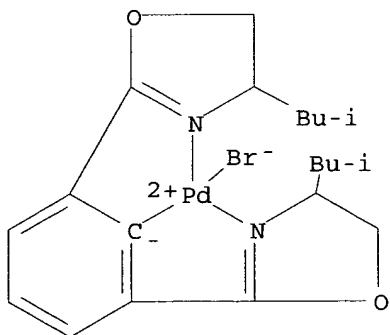


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RN 265127-67-1 HCAPLUS
 CN Palladium, [2,6-bis[(4S)-4,5-dihydro-4-(2-methylpropyl)-2-oxazolyl- κ N3]phenyl- κ C]bromo-, (SP-4-3)- (9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
 Section cross-reference(s): 21, 22, 67, 75
 IT **Michael reaction catalysts**
 (stereoselective; chiral cationic bis(oxazolinyll)palladium(II) complexes as catalysts for asym. Michael reaction)
 IT **Michael reaction**
 (stereoselective; chiral cationic bis(oxazolinyll)phenylpalladium(II) complexes as **catalysts** for asym. Michael reaction)
 IT **Asymmetric synthesis and induction**
 (using chiral cationic bis(oxazolinyll)palladium(II) complexes as catalysts for asym. Michael reactions to form chiral products)
 IT 78-94-4, 3-Buten-2-one, reactions 105-56-6, Ethyl cyanoacetate 107-13-1, 2-Propenenitrile, reactions 603-67-8, Diethyl nitromalonate 1572-99-2, Ethyl α -cyanopropionate 66476-82-2, tert-Butyl α -cyanopropionate
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 ([bis(oxazolinyll)phenyl]palladium(II) cationic complex-catalyzed asym. Michael reaction of)

- IT 162157-05-3, (S)-2-Ferrocenyl-4-benzyl-2-oxazoline
RL: RCT (Reactant); RACT (Reactant or reagent)
(benzylic deprotonation followed by reaction with acid)
- IT 196207-76-8P
RL: CAT (Catalyst use); PRP (Properties); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(crystal structure; preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)
- IT 196207-77-9P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as catalyst for asym. Michael reaction and substitution reaction with nitriles)
- IT 1273-84-3P, Ferrocenyl cyanide 4407-36-7P, (E)-Cinnamyl alcohol 99170-86-2P, 4,4-Bis(carboethoxy)-4-nitrobutanenitrile 143619-24-3P, (R)-Ethyl 2-cyano-2-methyl-5-oxohexanoate 143619-26-5P, (R)-tert-Butyl 2-cyano-2-methyl-5-oxohexanoate 181186-07-2P, 5-Cyano-5-(carboethoxy)nonane-2,8-dione 196207-74-6P 265127-68-2P 265127-71-7P, (R,R)-2-Methyl-1,3-bis(4-phenyl-2-oxazolin-2-yl)benzene 265127-72-8P 265127-80-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)
- IT 196207-80-4P 196207-82-6P 265127-73-9P 265127-74-0P 265127-76-2P 265127-78-4P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation of cationic [bis(oxazolinyl)phenyl]palladium(II) complexes as catalysts for asym. Michael reaction)
- IT 189632-52-8P 196207-70-2P 196207-71-3P 196207-72-4P 265127-67-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation of cationic palladium bis(oxazolinyl)benzene aquo complexes from)

REFERENCE COUNT: 90 THERE ARE 90 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 22 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1999:401284 HCAPLUS

DOCUMENT NUMBER: 131:170456

TITLE: Synthesis and Structure of Enantiomerically Pure Platinum Complexes of Phosphino-oxazolines and Their Use in Asymmetric Catalysis

AUTHOR(S): Blacker, A. John; Clarke, Matthew L.; Loft, Michael S.; Mahon, Mary F.; Williams, Jonathan M. J.

CORPORATE SOURCE: Huddersfield Works, Zeneca, Huddersfield, HD2 1FF, UK

SOURCE: Organometallics (1999), 18(15), 2867-2873

CODEN: ORGND7; ISSN: 0276-7333

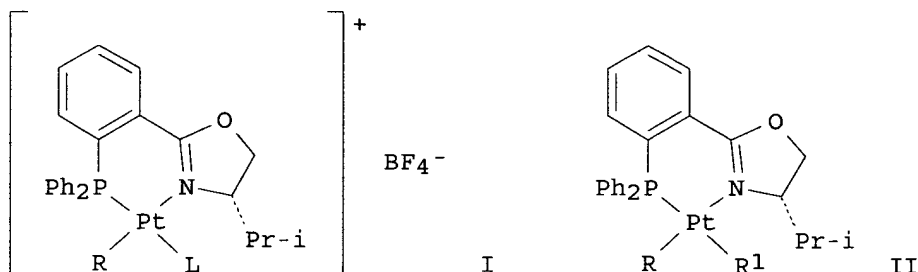
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 131:170456

GI



AB Novel organoplatinum complexes of the enantiomerically pure P, N ligand, (4*S*)-2-[2-(diphenylphosphino)phenyl]-4-isopropyl-1,3-oxazoline (e.g. I; L = ClCH₂Cl, R = Me (5a), Ph (5b)), were synthesized and shown to act as Lewis acids. These complexes consist of the bidentate P, N ligand, an achiral organic ligand, and a solvent ligand that can be readily displaced by organic substrates. The solvent ligand is situated *cis* to the N donor and, as such, is in a chiral pocket created by the oxazoline ring. The complexes are readily prepared from the known, and versatile, precursors (COD)PtR₂ (R = Me, Ph) and were obtained as single isomers. Two of the complexes II (R = R₁ = Ph (3b); R = Me, R₁ = Cl (4a)) have had their structures elucidated by x-ray crystallog. The cationic complexes 5a and 5b are enantioselective catalysts in the Michael reaction of α -cyano carboxylates with Me vinyl ketone. Complex 5a catalyzed the Diels Alder reaction of cyclopentadiene with 2-chloroacrylonitrile to give high conversion to a 7:1 mixture of *endo* and *exo* isomers of the resulting adduct with low enantioselectivity (ca. 10% ee).

ED Entered STN: 30 Jun 1999

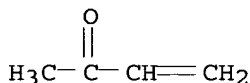
IT 78-94-4, Methyl vinyl ketone, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. Michael reaction with Et cyanopropionate catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)

RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)

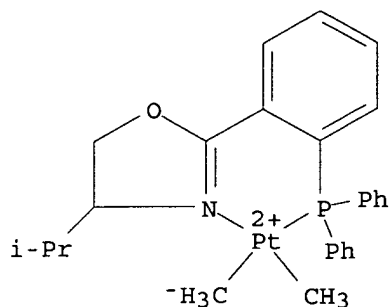


IT 239099-78-6P

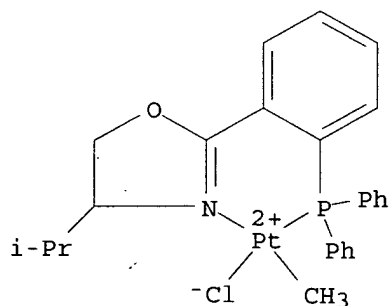
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and chlorination of)

RN 239099-78-6 HCAPLUS

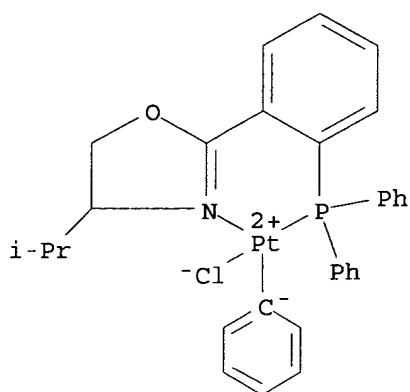
CN Platinum, [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]dimethyl-, (SP-4-3)-(9CI) (CA INDEX NAME)



IT 239099-80-0DP, petroleum ether solvate
 RL: PRP (Properties); SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation and crystal structure of)
 RN 239099-80-0 HCAPLUS
 CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-
 dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-2)-
 (9CI) (CA INDEX NAME)



IT 239099-81-1P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation and reaction with dichloromethane and silver
 tetrafluoroborate)
 RN 239099-81-1 HCAPLUS
 CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-
 dihydro-4-(1-methylethyl)oxazole-κN3]phenyl-, (SP-4-2)-
 (9CI) (CA INDEX NAME)



IT 239099-83-3P

RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)

(preparation as enantioselective Michael reaction catalysts for reaction of α -cyano carboxylates with Me vinyl ketone)

RN 239099-83-3 HCAPLUS

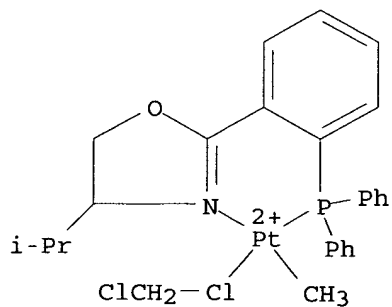
CN Platinum(1+), [(chloro- κ Cl)chloromethane] [(4S)-2-[2-(diphenylphosphino- κ P)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole- κ N3]methyl-, (SP-4-2)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 239099-82-2

CMF C26 H29 Cl2 N O P Pt

CCI CCS

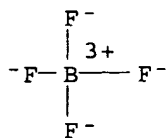


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 239099-85-5P

RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)

(preparation as enantioselective Michael reaction catalysts for reaction of α -cyano carboxylates with Me vinyl ketone)

RN 239099-85-5 HCAPLUS

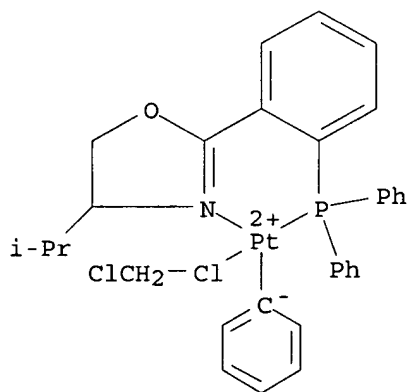
CN Platinum(1+), [(chloro- κ Cl)chloromethane] [(4S)-2-[2-(diphenylphosphino- κ P)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole- κ N3]phenyl-, (SP-4-2)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 239099-84-4

CMF C31 H31 Cl2 N O P Pt

CCI CCS

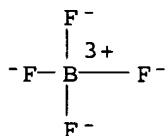


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS



IT 239099-87-7P 239099-89-9P 239099-91-3P

239099-93-5P

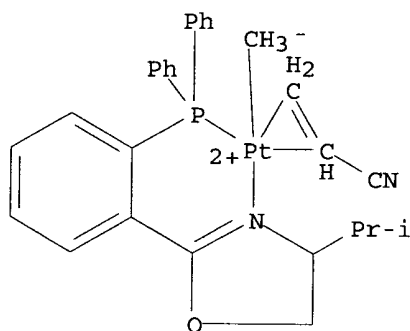
RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 239099-87-7 HCAPLUS
 CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl[(2,3-η)-2-propenenitrile]-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

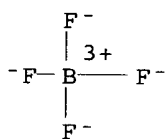
CM 1

CRN 239099-86-6
 CMF C28 H30 N2 O P Pt
 CCI CCS



CM 2

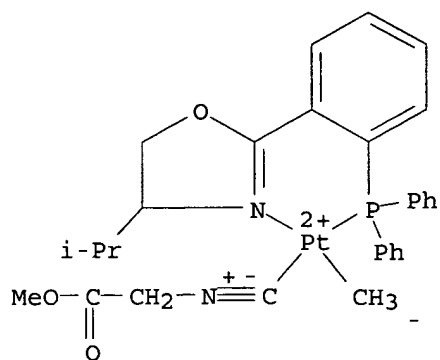
CRN 14874-70-5
 CMF B F4
 CCI CCS



RN 239099-89-9 HCAPLUS
 CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl[methyl(isocyano-κC)acetate]-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 239099-88-8
 CMF C29 H32 N2 O3 P Pt
 CCI CCS

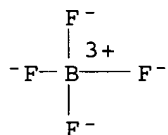


CM 2

CRN 14874-70-5

CMF B F4

CCI CQS



RN 239099-91-3 HCAPLUS

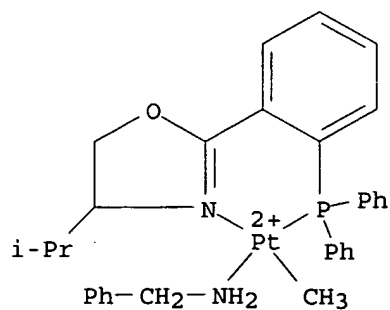
CN Platinum(1+), (benzenemethanamine) [(4S)-2-[2-(diphenylphosphino- κ P)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole- κ N3]methyl-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 239099-90-2

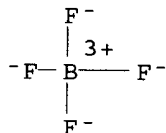
CMF C32 H36 N2 O P Pt

CCI CCS



CM 2

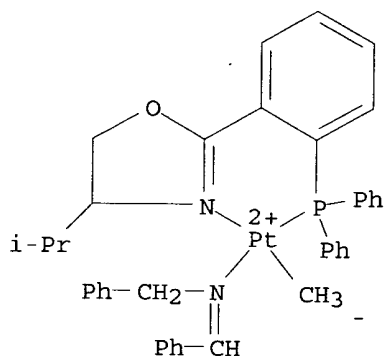
CRN 14874-70-5
CMF B F4
CCI CCS



RN 239099-93-5 HCAPLUS
CN Platinum(1+), [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl [N-(phenylmethylene)benzenemethanamine]-, (SP-4-3)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

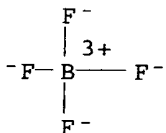
CM 1

CRN 239099-92-4
CMF C39 H40 N2 O P Pt
CCI CCS



CM 2

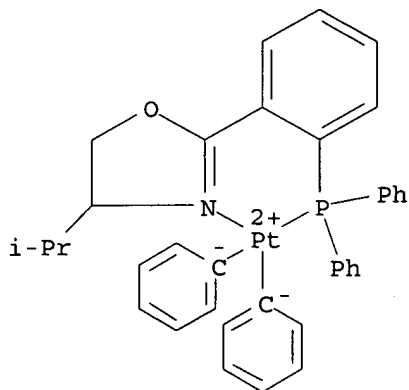
CRN 14874-70-5
CMF B F4
CCI CCS



IT 239099-79-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure, and chlorination of)

RN 239099-79-7 HCAPLUS

CN Platinum, [(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]diphenyl-, (SP-4-3)-(9CI) (CA INDEX NAME)

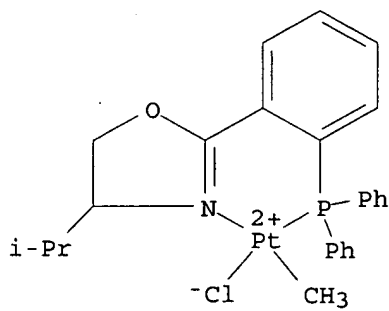


IT 239099-80-0P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, mol. structure, and reaction with dichloromethane and silver tetrafluoroborate)

RN 239099-80-0 HCAPLUS

CN Platinum, chloro[(4S)-2-[2-(diphenylphosphino-κP)phenyl]-4,5-dihydro-4-(1-methylethyl)oxazole-κN3]methyl-, (SP-4-2)-(9CI) (CA INDEX NAME)



CC 29-13 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 23, 24, 67, 75

IT **Asymmetric synthesis and induction**

(in Michael reaction of α-cyano carboxylates with Me vinyl ketone catalyzed by organoplatinum (phosphinophenyl)oxazoline enantiomerically pure complexes)

IT **Michael reaction**

(stereoselective; of α-cyano carboxylates with Me vinyl ketone catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)

IT **Michael reaction catalysts**

(stereoselective; organoplatinum (phosphinophenyl)oxazoline complexes for reaction of α-cyano carboxylates with Me

vinyl ketone)

IT 78-94-4, Methyl vinyl ketone, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. Michael reaction with Et cyanopropionate catalyzed by organoplatinum (phosphinophenyl)oxazoline complexes)

IT 239099-78-6P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and chlorination of)

IT 239099-80-0DP, petroleum ether solvate
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(preparation and crystal structure of)

IT 239099-81-1P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation and reaction with dichloromethane and silver tetrafluoroborate)

IT 239099-83-3P
RL: CAT (Catalyst use); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α -cyano carboxylates with Me vinyl ketone)

IT 239099-85-5P
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as enantioselective Michael reaction catalysts for reaction of α -cyano carboxylates with Me vinyl ketone)

IT 143619-24-3P 239099-87-7P 239099-89-9P
239099-91-3P 239099-93-5P
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT 239099-79-7P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, crystal structure, and chlorination of)

IT 239099-80-0P
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)
(preparation, mol. structure, and reaction with dichloromethane and silver tetrafluoroborate)

REFERENCE COUNT: 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L93 ANSWER 23 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1998:270307 HCAPLUS
DOCUMENT NUMBER: 129:67541
TITLE: A New Palladium(II)-Catalyzed Asymmetric Chlorohydrin Synthesis
AUTHOR(S): El-Qisairi, Arab; Hamed, Othman; Henry, Patrick M.
CORPORATE SOURCE: Department of Chemistry, Loyola University of Chicago, Chicago, IL, 60626, USA
SOURCE: Journal of Organic Chemistry (1998), 63(9), 2790-2791
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal

LANGUAGE: English
 OTHER SOURCE(S): CASREACT 129:67541

AB Previous studies show that addition of a neutral ligand, L, to the coordination sphere of PdCl_2 to give PdCl_2L under the conditions of the Wacker reaction changes the product from exclusively acetaldehyde to mainly 2-chloroethanol. Oxidation of α -olefins with a catalyst in which the neutral ligand is a chiral amine or phosphine should result in chiral chlorohydrins. Oxidation of propene with a catalyst containing a chiral amine produced propylene chlorohydrin with an optical purity of 10-15% ee. Catalysts containing chiral diphosphines should increase the optical purities. However, the neutral catalyst, $\text{PdCl}_2(\text{L}^*-\text{L}^*)$ is insol. in the reaction media. The solution to this problem involved two distinct approaches. The first approach used monometallic catalysts containing sulfonated p-Tol-BINAP ligands to increase solubility. Optical purities ranged from 46% ee for propene to 76% ee for allyl Ph ether. The second approach used bimetallic catalysts containing a β -triketone and bridging chiral phosphine. Optical purities were higher for this system. The % ee's were >80% for all olefins tested. The highest were observed for propene with 94% ee and allyl Ph ether with 93% ee.

ED Entered STN: 13 May 1998

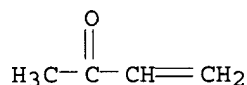
IT 78-94-4, 3-Buten-2-one, reactions 520-45-6,
 Dehydroacetic acid 14220-64-5,

Bis(benzonitrile)dichloropalladium

RL: RCT (Reactant); RACT (Reactant or reagent)
 (palladium(II)-catalyzed asym. chlorohydrin synthesis)

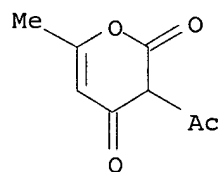
RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



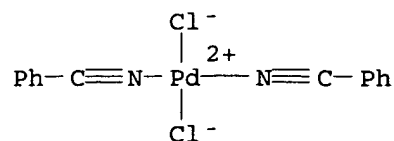
RN 520-45-6 HCAPLUS

CN 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl- (8CI, 9CI) (CA INDEX NAME)



RN 14220-64-5 HCAPLUS

CN Palladium, bis(benzonitrile)dichloro- (8CI, 9CI) (CA INDEX NAME)



CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 23

IT **Asymmetric synthesis and induction**
(palladium(II)-catalyzed asym. chlorohydrin synthesis)

IT 75-05-8, Acetonitrile, reactions 78-94-4, 3-Buten-2-one,
reactions 90-15-3, 1-Naphthol 93-58-3, Methyl benzoate
106-95-6, Allyl bromide, reactions 109-67-1, 1-Pentene
115-07-1, 1-Propene, reactions 123-54-6, 2,4-Pentanedione,
reactions 520-45-6, Dehydroacetic acid 592-41-6,
1-Hexene, reactions 1746-13-0, Allyl phenyl ether 7440-05-3,
Palladium, reactions 10025-98-6, Dipotassium
tetrachloropalladate 14220-64-5,
Bis(benzonitrile)dichloropalladium 14635-75-7, Nitrosonium
tetrafluoroborate 37676-25-8 76189-56-5, (S)-BINAP
86342-85-0 99646-28-3
RL: RCT (Reactant); RACT (Reactant or reagent)
(palladium(II)-catalyzed asym. chlorohydrin synthesis)

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 24 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1997:474075 HCAPLUS

DOCUMENT NUMBER: 127:161626

TITLE: Asymmetric total syntheses of (+)-coronafacic
acid and (+)-coronatine, phytotoxins isolated
from Pseudomonas syringae pathovars

AUTHOR(S): Nara, Shinji; Toshima, Hiroaki; Ichihara,
Akitami

CORPORATE SOURCE: Department Bioscience Chemistry, Faculty
Agriculture, Hokkaido University, Sapporo,
060, Japan

SOURCE: Tetrahedron (1997), 53(28),
9509-9524
CODEN: TETRAB; ISSN: 0040-4020

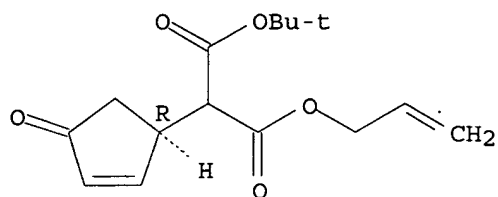
PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:161626

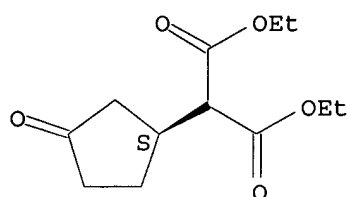
GI



RN 193530-87-9 HCAPLUS

CN Propanedioic acid, [(1S)-3-oxocyclopentyl]-, diethyl ester (9CI)
(CA INDEX NAME)

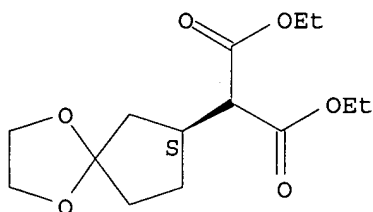
Absolute stereochemistry. Rotation (-).



RN 193530-88-0 HCAPLUS

CN Propanedioic acid, (7S)-1,4-dioxaspiro[4.4]non-7-yl-, diethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 26-9 (Biomolecules and Their Synthetic Analogs)

IT **Asymmetric synthesis and induction**

(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)

IT 105-53-3, Diethyl malonate 922-63-4, 2-Ethylacrolein
930-30-3, 2-Cyclopentenone 59995-48-1 62457-60-7
166826-51-3 183253-55-6

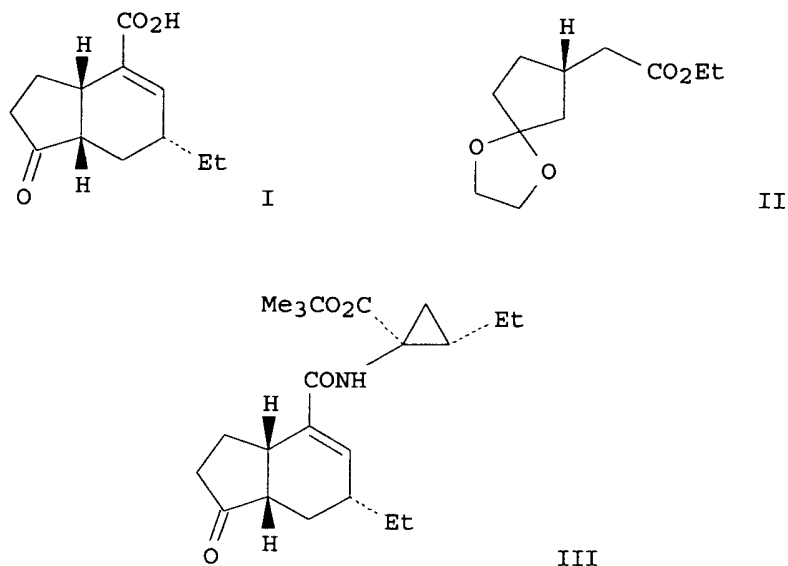
RL: RCT (Reactant); RACT (Reactant or reagent)

(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)

IT 42726-73-8P 79405-48-4P 93306-08-2P 132665-05-5P
134209-82-8P 183115-24-4P 183115-27-7P 189506-59-0P
189506-61-4P 190073-22-4P 193530-85-7P 193530-86-8P
193530-87-9P 193530-88-0P 193530-90-4P
193530-91-5P 193530-92-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(asym. total syntheses of (+)-coronafacic acid and
(+)-coronatine)



AB Asym. total synthesis of (+)-coronafacic acid (I), was accomplished via intramol. 1,6-conjugate addition as the key step. The chiral ester (+)-II was prepared via two approaches: starting from (R)-(+)-4-acetoxy-2-cyclopenten-1-one, and using catalytic asym. Michael reactions promoted by heterobimetallic BINOL complexes. Coupling between (+)-I and the protected coronamic acid and subsequent deprotection by hydrogenolysis provided (+)-coronatine (III). This is the first asym. total synthesis of (+)-III.

ED Entered STN: 30 Jul 1997

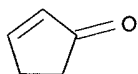
IT 930-30-3, 2-Cyclopentenone

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(asym. total syntheses of (+)-coronafacic acid and (+)-coronatine)

RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



IT 193530-86-8P 193530-87-9P 193530-88-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**

(asym. total syntheses of (+)-coronafacic acid and (+)-coronatine)

RN 193530-86-8 HCAPLUS

CN Propanedioic acid, (4-oxo-2-cyclopenten-1-yl)-, 1,1-dimethylethyl 2-propenyl ester, (1R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L93 ANSWER 25 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:513724 HCAPLUS

DOCUMENT NUMBER: 125:220828

TITLE: Michael Reaction of Stabilized Carbon
Nucleophiles Catalyzed by [RuH₂(PPh₃)₄]

AUTHOR(S): Gomez-Bengoa, Enrique; Cuerva, Juan M.; Mateo,
Cristina; Echavarren, Antonio M.

CORPORATE SOURCE: Departamento de Quimica Organica, Universidad
Autonoma de Madrid, Madrid, 28049, Spain

SOURCE: Journal of the American Chemical Society (
1996), 118(36), 8553-8565

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:220828

AB The Michael reaction of active methylene compds. lacking cyano
groups such as malonates, β -ketoesters, 1,3-diketones,
1,1-disulfones, nitro compds., Meldrum acid, and anthrone with
common acceptors proceeds in acetonitrile solution in the presence of
[RuH₂(PPh₃)₄] as the catalyst. Cyano acetates, more acidic than
malonates in organic solvents, are also excellent substrates for this
reaction. In a number of cases, intramol. aldol reactions catalyzed
by [RuH₂(PPh₃)₄] were also observed as side reactions. Catalysis by
other ruthenium and rhodium complexes has been examined. Selectivity
studies performed with malonate and disulfone donors indicate that
the catalyst selectively activates Michael donors that can
coordinate with ruthenium(II). Addnl., it has been shown that the
reaction requires the presence of free phosphine. Therefore, the
Michael reaction of stabilized enolates appears to be a ruthenium-
and phosphine-catalyzed reaction. From a practical point of view,
the use of readily prepared [RuH₂(PPh₃)₄] as the catalyst in
acetonitrile provided the best solution for the Michael reaction of
active methylene compds.

ED Entered STN: 28 Aug 1996

IT 40988-90-7 132751-57-6

RL: CAT (Catalyst use); USES (Uses)

(Michael reaction of stabilized carbon nucleophiles catalyzed
by [RuH₂(PPh₃)₄] and related compds.)

RN 40988-90-7 HCAPLUS

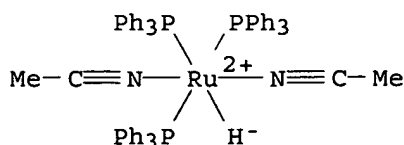
CN Ruthenium(1+), bis(acetonitrile)hydrotris(triphenylphosphine)-,
(OC-6-21)-, hexafluorophosphate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 48245-15-4

CMF C58 H52 N2 P3 Ru

CCI CCS

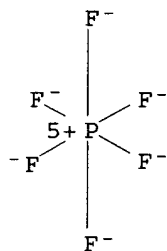


CM 2

CRN 16919-18-9

CMF F6 P

CCI CCS



RN 132751-57-6 HCAPLUS

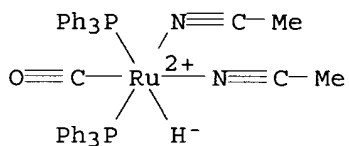
CN Ruthenium(1+), bis(acetonitrile)carbonylhydrobis(triphenylphosphine)-, (OC-6-14)-, tetrafluoroborate(1-) (9CI) (CA INDEX NAME)

CM 1

CRN 47868-22-4

CMF C41 H37 N2 O P2 Ru

CCI CCS

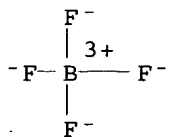


CM 2

CRN 14874-70-5

CMF B F4

CCI CCS

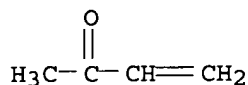
IT 78-94-4, Methyl vinyl ketone, reactions 930-68-7
, 2-Cyclohexen-1-one 121730-78-7

RL: RCT (Reactant); RACT (Reactant or reagent)

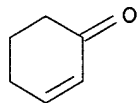
(Michael reaction of stabilized carbon nucleophiles catalyzed
by [RuH2(PPh3)4] and related compds.)

RN 78-94-4 HCAPLUS

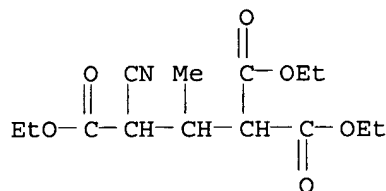
CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



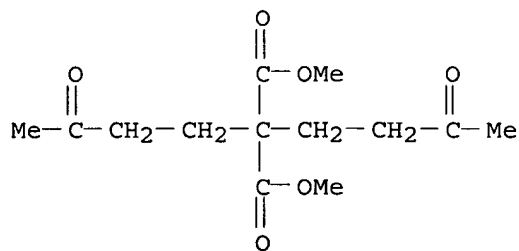
RN 930-68-7 HCAPLUS
 CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



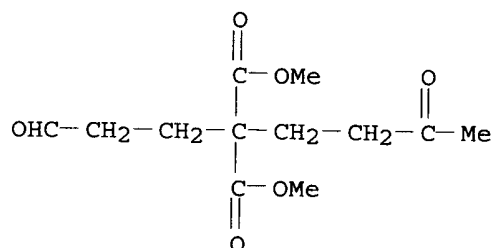
RN 121730-78-7 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl ester
 (9CI) (CA INDEX NAME)



IT 151920-47-7P 181186-01-6P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (Michael reaction of stabilized carbon nucleophiles catalyzed
 by [RuH₂(PPh₃)₄] and related compds.)
 RN 151920-47-7 HCAPLUS
 CN Propanedioic acid, bis(3-oxobutyl)-, dimethyl ester (9CI) (CA
 INDEX NAME)



RN 181186-01-6 HCAPLUS
 CN Propanedioic acid, (3-oxobutyl)(3-oxopropyl)-, dimethyl ester
 (9CI) (CA INDEX NAME)

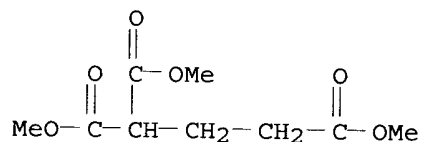


IT 1733-16-0P 25112-78-1P 33646-18-3P
 42593-60-2P 59104-44-8P 95929-65-0P
 181185-88-6P 181185-89-7P 181185-90-0P
 181185-92-2P 181185-93-3P 181185-94-4P
 181185-95-5P 181185-96-6P 181186-02-7P
 181186-03-8P 181186-04-9P 181186-05-0P
 181186-06-1P 181377-47-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (Michael reaction of stabilized carbon nucleophiles catalyzed
 by [RuH₂(PPh₃)₄] and related compds.)

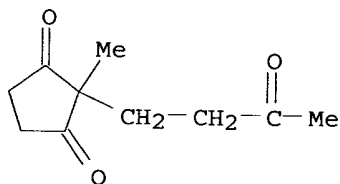
RN 1733-16-0 HCAPLUS

CN 1,1,3-Propanetricarboxylic acid, trimethyl ester (7CI, 8CI, 9CI)
 (CA INDEX NAME)



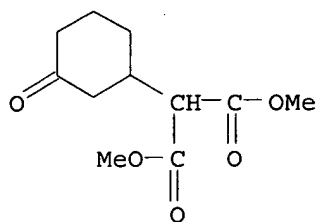
RN 25112-78-1 HCAPLUS

CN 1,3-Cyclopentanedione, 2-methyl-2-(3-oxobutyl)- (6CI, 8CI, 9CI)
 (CA INDEX NAME)

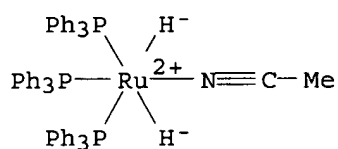


RN 33646-18-3 HCAPLUS

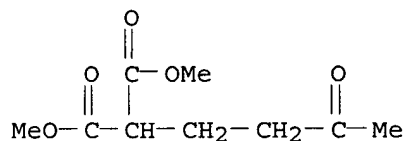
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA
 INDEX NAME)



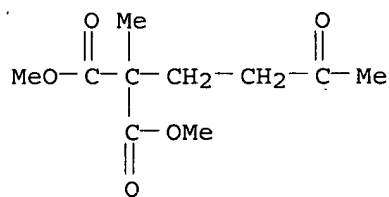
RN 42593-60-2 HCAPLUS
 CN Ruthenium, (acetonitrile)dihydrotris(triphenylphosphine) - (9CI)
 (CA INDEX NAME)



RN 59104-44-8 HCAPLUS
 CN Propanedioic acid, (3-oxobutyl)-, dimethyl ester (9CI) (CA INDEX NAME)

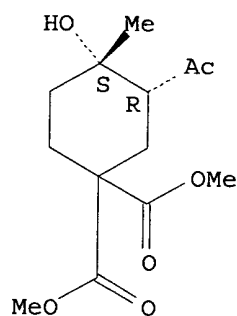


RN 95929-65-0 HCAPLUS
 CN Propanedioic acid, methyl(3-oxobutyl)-, dimethyl ester (9CI) (CA INDEX NAME)



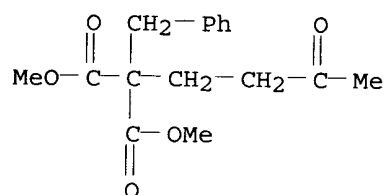
RN 181185-88-6 HCAPLUS
 CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-4-methyl-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

Relative stereochemistry.



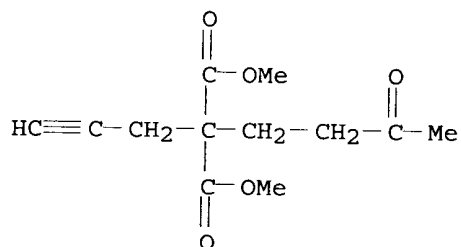
RN 181185-89-7 HCAPLUS

CN Propanedioic acid, (3-oxobutyl)(phenylmethyl)-, dimethyl ester
(9CI) (CA INDEX NAME)



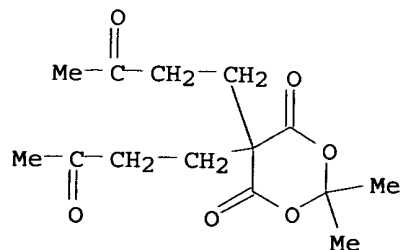
RN 181185-90-0 HCAPLUS

CN Propanedioic acid, (3-oxobutyl)-2-propynyl-, dimethyl ester (9CI)
(CA INDEX NAME)



RN 181185-92-2 HCAPLUS

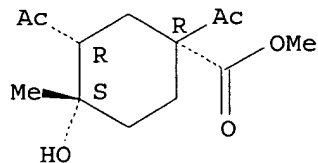
CN 1,3-Dioxane-4,6-dione, 2,2-dimethyl-5,5-bis(3-oxobutyl)- (9CI)
(CA INDEX NAME)



RN 181185-93-3 HCAPLUS

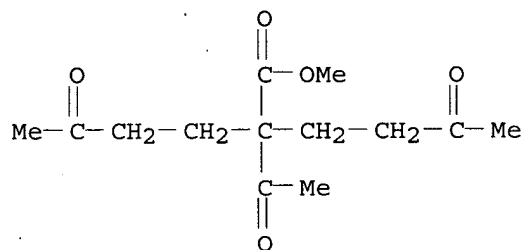
CN Cyclohexanecarboxylic acid, 1,3-diacetyl-4-hydroxy-4-methyl-, methyl ester, (1 α ,3 α ,4 α)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



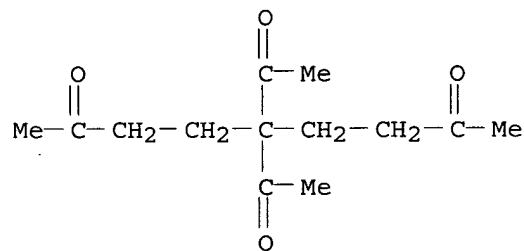
RN 181185-94-4 HCAPLUS

CN Hexanoic acid, 2-acetyl-5-oxo-2-(3-oxobutyl)-, methyl ester (9CI) (CA INDEX NAME)



RN 181185-95-5 HCAPLUS

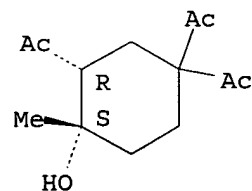
CN 2,8-Nonanedione, 5,5-diacetyl- (9CI) (CA INDEX NAME)



RN 181185-96-6 HCAPLUS

CN Ethanone, 1,1',1''-[(1R,6S)-6-hydroxy-6-methyl-1-cyclohexanyl-3-ylidene]tris-, rel- (9CI) (CA INDEX NAME)

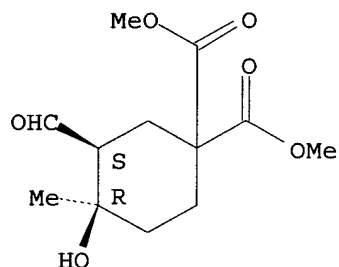
Relative stereochemistry.



RN 181186-02-7 HCAPLUS

CN 1,1-Cyclohexanedicarboxylic acid, 3-formyl-4-hydroxy-4-methyl-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

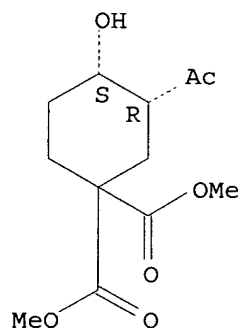
Relative stereochemistry.



RN 181186-03-8 HCAPLUS

CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-, dimethyl ester, cis- (9CI) (CA INDEX NAME)

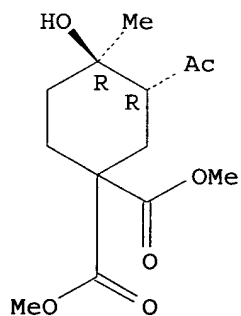
Relative stereochemistry.



RN 181186-04-9 HCAPLUS

CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-4-methyl-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

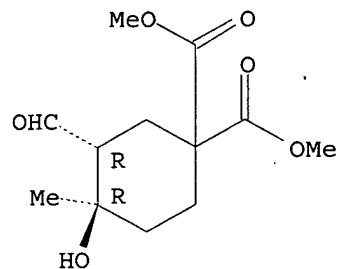
Relative stereochemistry.



RN 181186-05-0 HCAPLUS

CN 1,1-Cyclohexanedicarboxylic acid, 3-formyl-4-hydroxy-4-methyl-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

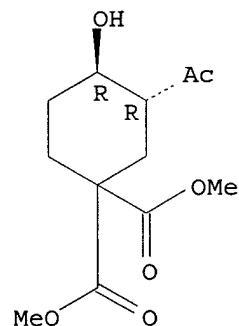
Relative stereochemistry.



RN 181186-06-1 HCAPLUS

CN 1,1-Cyclohexanedicarboxylic acid, 3-acetyl-4-hydroxy-, dimethyl ester, trans- (9CI) (CA INDEX NAME)

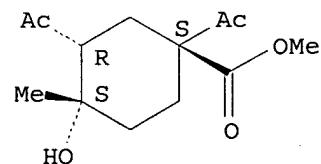
Relative stereochemistry.



RN 181377-47-9 HCAPLUS

CN Cyclohexanecarboxylic acid, 1,3-diacetyl-4-hydroxy-4-methyl-, methyl ester, (1α,3β,4β)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



CC 21-2 (General Organic Chemistry)

IT Michael reaction

Michael reaction catalysts

(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH₂(PPh₃)₄] and related compds.)

IT 603-32-7, Triphenylarsine 603-35-0, Triphenylphosphine, uses
 998-40-3, Tributylphosphine 2622-14-2, Tricyclohexylphosphine
 12150-46-8, Dppf 15529-49-4 22172-51-6 22337-78-6
 40988-90-7 61521-25-3 74735-07-2 114595-94-7
 132724-29-9 132751-57-6 156734-49-5 157931-51-6
 181377-46-8

RL: CAT (Catalyst use); USES (Uses)

(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH₂(PPh₃)₄] and related compds.)

IT 78-94-4, Methyl vinyl ketone, reactions 79-24-3, Nitroethane 86-73-7, Fluorene 90-44-8, Anthrone 96-33-3, Methyl acrylate 105-45-3, Methyl 3-oxobutyrate 105-56-6, Ethyl cyanoacetate 107-02-8, 2-Propenal, reactions 107-13-1, 2-Propenenitrile, reactions 108-59-8, Dimethyl malonate 123-54-6, 2,4-Pentanedione, reactions 538-58-9, Dibenzylideneacetone 609-02-9, Dimethyl methylmalonate 624-49-7, Dimethyl fumarate 765-69-5 930-68-7, 2-Cyclohexen-1-one 2033-24-1 3406-02-8, Bis(phenylsulfonyl)methane 4170-30-3, Crotonaldehyde 5535-48-8, Phenyl vinyl sulfone 49769-78-0, Dimethyl benzylmalonate 50765-99-6 54083-06-6 95124-07-5 121730-78-7 133817-97-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH₂(PPh₃)₄] and related compds.)

IT 72473-15-5P 151920-47-7P 181186-01-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH₂(PPh₃)₄] and related compds.)

IT 1733-16-0P 19766-36-0P 25112-78-1P 33646-18-3P 35223-72-4P 42593-60-2P 55525-27-4P 59104-44-8P 81794-16-3P 87625-87-4P 95929-65-0P 136917-89-0P 173593-86-7P 181185-88-6P 181185-89-7P 181185-90-0P 181185-91-1P 181185-92-2P 181185-93-3P 181185-94-4P 181185-95-5P 181185-96-6P 181185-97-7P 181185-98-8P 181185-99-9P 181186-00-5P 181186-02-7P 181186-03-8P 181186-04-9P 181186-05-0P 181186-06-1P 181186-07-2P 181186-08-3P 181186-09-4P 181186-10-7P 181186-11-8P 181186-14-1P 181377-43-5P 181377-47-9P 181377-48-0P 181377-49-1P 181377-50-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(Michael reaction of stabilized carbon nucleophiles catalyzed by [RuH₂(PPh₃)₄] and related compds.)

L93 ANSWER 26 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:380129 HCAPLUS

DOCUMENT NUMBER: 125:86908

TITLE: A New Catalyst for a Pd Catalyzed Alder Ene Reaction. A Total Synthesis of (+)-Cassioid

AUTHOR(S): Trost, Barry M.; Li, Yong

CORPORATE SOURCE: Department of Chemistry, Stanford University, Stanford, CA, 94305, USA

SOURCE: Journal of the American Chemical Society (1996), 118(28), 6625-6633

CODEN: JACSAT; ISSN: 0002-7863

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 125:86908

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT

AB The scope of the palladium catalyzed cycloisomerization of enynes, e.g. alkyne I to cyclohexanone II, in an Alder ene type fashion that led to a new catalytic system was explored in the context of a synthetic strategy to the antiulcerogenic agent (+)-cassiol (III). In a model study, the effect of six-membered ring formation, the presence of a carbonyl group in the tether, and the steric hindrance of the alkene conspire to prevent the cycloisomerization under the "standard" conditions. Two variables proved key in the development of a new catalytic system that has proven to be effective, the absence of traditional ligands and the choice of acid. An effective synthesis of (+)-cassiol (III) was accomplished in which this new reaction played a key. A lipase served to introduce the chirality, and a palladium(0) catalyzed reaction was important in elaborating a side chain. The final adjustment of oxidation level made advantageous use of a platinum catalyzed enone hydrosilylation.

ED Entered STN: 02 Jul 1996

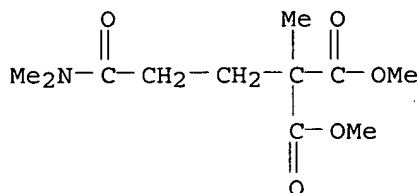
IT 178559-14-3P

RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)

(total synthesis of (+)-cassiol via palladium-catalyzed Alder ene reaction)

RN 178559-14-3 HCAPLUS

CN Propanedioic acid, [3-(dimethylamino)-3-oxopropyl]methyl-, dimethyl ester (9CI) (CA INDEX NAME)



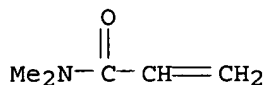
IT 2680-03-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(total synthesis of (+)-cassiol via palladium-catalyzed Alder ene reaction)

RN 2680-03-7 HCAPLUS

CN 2-Propenamamide, N,N-dimethyl- (9CI) (CA INDEX NAME)



CC 30-15 (Terpenes and Terpenoids)

Section cross-reference(s): 26, 33

IT Asymmetric synthesis and induction

(total synthesis of (+)-cassiol via palladium-catalyzed Alder ene reaction)

IT 178559-14-3P
RL: BPR (Biological process); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process); RACT (Reactant or reagent)
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

IT 108-59-8, Dimethyl malonate 609-02-9, Dimethyl methylmalonate 1066-54-2, (Trimethylsilyl)acetylene 2680-03-7 5497-67-6, 2,2-Dimethyl-4-pentenal
RL: RCT (Reactant); RACT (Reactant or reagent)
(total synthesis of(+)-cassiol via palladium-catalyzed Alder ene reaction)

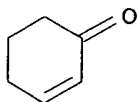
L93 ANSWER 27 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 1996:259869 HCAPLUS
DOCUMENT NUMBER: 125:32888
TITLE: Asymmetric Michael Addition of Malonate Anions to Prochiral Acceptors Catalyzed by L-Proline Rubidium Salt
AUTHOR(S): Yamaguchi, Masahiko; Shiraishi, Tai; Hirama, Masahiro
CORPORATE SOURCE: Graduate School of Science, Tohoku University, Sendai, 980-77, Japan
SOURCE: Journal of Organic Chemistry (1996), 61(10), 3520-30
CODEN: JOCEAH; ISSN: 0022-3263
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 125:32888

AB L-Proline rubidium salt catalyzes the asym. Michael addition of malonate anions to prochiral enones and enals. This method can be applied to a wide range of substrates to give adducts with a predictable absolute configuration: (S)-adducts from (E)-enones/enals and (R)-adducts from cyclic (Z)-enones. Both the secondary amine moiety and the carboxylate moiety are critical for the catalytic activity and asym. induction. Varying the counteranion also affects the reaction course. High enantiomeric excesses were attained when di-tert-Bu malonate was added to (E)-enones in the presence of CsF. The stereochem. of the Michael reaction indicates that asym. induction takes place via enantioface discrimination involving the acceptor α -carbon atom rather than the β -carbon atom.

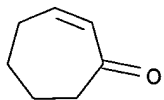
ED Entered STN: 03 May 1996

IT 930-68-7, 2-Cyclohexenone 1121-66-0, 2-Cycloheptenone 3102-33-8 32397-56-1 50396-87-7
RL: RCT (Reactant); RACT (Reactant or reagent)
(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

RN 930-68-7 HCAPLUS
CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)

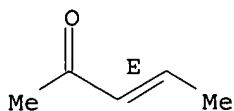


RN 1121-66-0 HCAPLUS
CN 2-Cyclohepten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



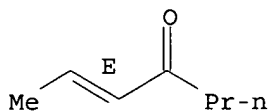
RN 3102-33-8 HCAPLUS
CN 3-Penten-2-one, (3E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



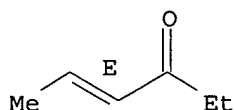
RN 32397-56-1 HCAPLUS
CN 2-Hepten-4-one, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



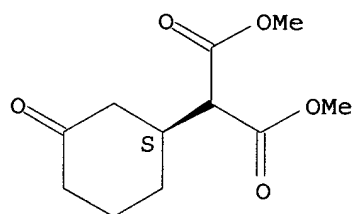
RN 50396-87-7 HCAPLUS
CN 4-Hexen-3-one, (4E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



IT 154194-50-0P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)
(asym. Michael addition of malonate anions to prochiral acceptors
catalyzed by L-proline rubidium salt)
RN 154194-50-0 HCAPLUS
CN Propanedioic acid, [(1S)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

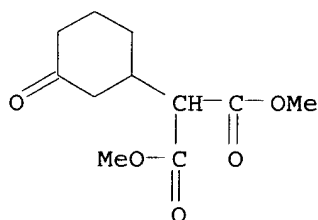


IT 33646-18-3P 177722-12-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(asym. Michael addition of malonate anions to prochiral acceptors
catalyzed by L-proline rubidium salt)

RN 33646-18-3 HCAPLUS

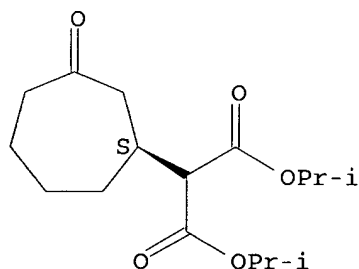
CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA
INDEX NAME)



RN 177722-12-2 HCAPLUS

CN Propanedioic acid, (3-oxocycloheptyl)-, bis(1-methylethyl) ester,
(S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 151600-45-2P 151600-46-3P 164931-77-5P

164931-78-6P 177722-13-3P 177722-18-8P

177722-20-2P 177722-22-4P 177722-26-8P

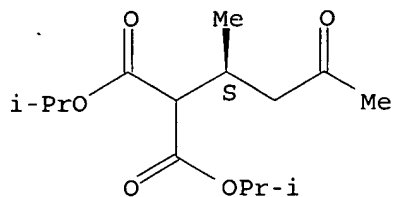
177722-27-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 151600-45-2 HCAPLUS

CN Propanedioic acid, (1-methyl-3-oxobutyl)-, bis(1-methylethyl)
ester, (S)- (9CI) (CA INDEX NAME)

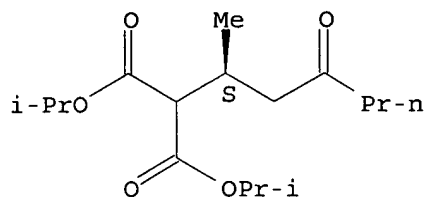
Absolute stereochemistry. Rotation (-).



RN 151600-46-3 HCAPLUS

CN Propanedioic acid, (1-methyl-3-oxohexyl)-, bis(1-methylethyl) ester, (S)- (9CI) (CA INDEX NAME)

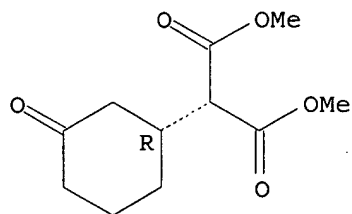
Absolute stereochemistry.



RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI) (CA INDEX NAME)

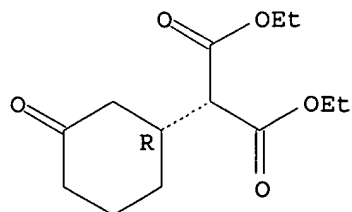
Absolute stereochemistry. Rotation (+).



RN 164931-78-6 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI) (CA INDEX NAME)

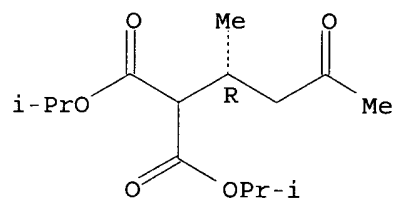
Absolute stereochemistry. Rotation (+).



RN 177722-13-3 HCAPLUS

CN Propanedioic acid, (1-methyl-3-oxobutyl)-, bis(1-methylethyl) ester, (R)- (9CI) (CA INDEX NAME)

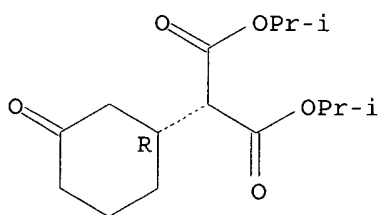
Absolute stereochemistry.



RN 177722-18-8 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)

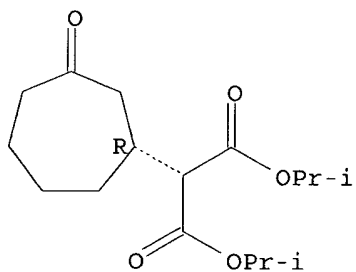
Absolute stereochemistry. Rotation (+).



RN 177722-20-2 HCAPLUS

CN Propanedioic acid, (3-oxocycloheptyl)-, bis(1-methylethyl) ester, (R)- (9CI) (CA INDEX NAME)

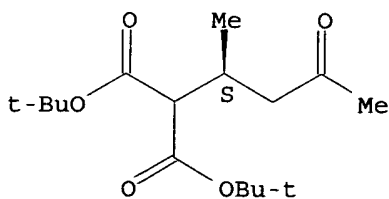
Absolute stereochemistry.



RN 177722-22-4 HCAPLUS

CN Propanedioic acid, [(1S)-1-methyl-3-oxobutyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

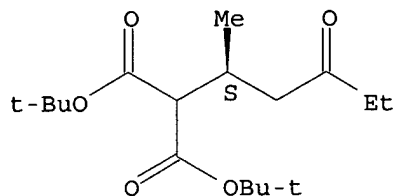
Absolute stereochemistry.



RN 177722-26-8 HCAPLUS

CN Propanedioic acid, (1-methyl-3-oxopentyl)-, bis(1,1-dimethylethyl) ester, (S)- (9CI) (CA INDEX NAME)

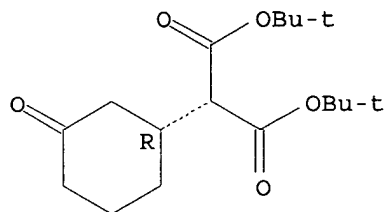
Absolute stereochemistry.



RN 177722-27-9 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, bis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



CC 21-2 (General Organic Chemistry)

IT **Asymmetric synthesis and induction****Michael reaction**

(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

IT **Michael reaction catalysts**

RL: CAT (Catalyst use); USES (Uses)

(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

IT 79-46-9, 2-Nitropropane 105-53-3, Diethyl malonate 108-59-8,

Dimethyl malonate 110-52-1, 1,4-Dibromobutane 123-73-9

541-16-2, Di-tert-butyl malonate 627-05-4, 1-Nitrobutane

930-68-7, 2-Cyclohexenone 1121-66-0,

2-Cycloheptenone 1694-31-1, tert-Butyl acetoacetate 1896-62-4

3102-33-8 6221-50-7 6728-26-3 13195-64-7,

Diisopropyl malonate 15014-25-2, Dibenzyl malonate 18402-83-0

23356-96-9, L-Prolinol 25112-78-1 32397-56-1

50396-87-7 56161-62-7 56345-01-8, (E)-2-

Cyclopentadecenone

RL: RCT (Reactant); **RACT (Reactant or reagent)**

(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

IT 33879-04-8P 84308-30-5P 151600-48-5P 154194-50-0P

177722-17-7P 177770-85-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); **RACT (Reactant or reagent)**

(asym. Michael addition of malonate anions to prochiral acceptors catalyzed by L-proline rubidium salt)

IT 33646-18-3P 63975-98-4P, (S)-(+)-Muscone 108329-93-7P

177722-12-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (asym. Michael addition of malonate anions to prochiral acceptors
 catalyzed by L-proline rubidium salt)

IT 17553-86-5P 89393-67-9P 96634-75-2P 108056-65-1P
151600-45-2P 151600-46-3P 151600-47-4P
 151600-51-0P 160012-11-3P 160012-12-4P 160012-13-5P
 160012-14-6P 160622-04-8P 160632-29-1P 164931-75-3P
164931-77-5P 164931-78-6P 177722-13-3P
 177722-14-4P 177722-15-5P 177722-16-6P **177722-18-8P**
 177722-19-9P **177722-20-2P** 177722-21-3P
177722-22-4P 177722-23-5P 177722-24-6P 177722-25-7P
177722-26-8P 177722-27-9P 177722-28-0P
 177722-29-1P 177722-30-4P 177722-31-5P 177770-89-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

L93 ANSWER 28 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1996:71012 HCAPLUS

DOCUMENT NUMBER: 124:231881

TITLE: A new multifunctional heterobimetallic
 asymmetric catalyst for Michael additions and
 tandem Michael-aldol reactions

AUTHOR(S): Arai, Takayoshi; Sasai, Hiroaki; Aoe,
 Kei-ichi; Okamura, Kimio; Date, Tadamasu;
 Shibasaki, Masakatsu

CORPORATE SOURCE: Fac. Pharmaceutical Sci., Univ. Tokyo, Tokyo,
 113, Japan

SOURCE: Angewandte Chemie, International Edition in
 English (1996), 35(1), 104-6
 CODEN: ACIEAY; ISSN: 0570-0833

PUBLISHER: VCH

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:231881

AB AllLi-BINOL complex was prepared from (R)-BINOL, diisobutylaluminum
 hydride, and BuLi and examined as a catalyst for Michael and
 Michael-aldol reactions of 2-cyclopentenone and 2-cyclohexenone.
 The structure of the product obtained from AllLi-BINOL and
 2-cyclohexenone was determined by X-ray anal.

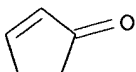
ED Entered STN: 01 Feb 1996

IT 930-30-3, 2-Cyclopentenone 930-68-7,
 2-Cyclohexenone

RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (aluminum-BINOL complex as asym. catalyst for Michael addns.
 and tandem Michael-aldol reactions)

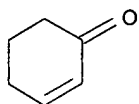
RN 930-30-3 HCAPLUS

CN 2-Cyclopenten-1-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



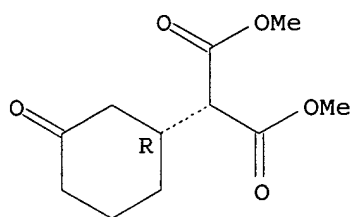
IT 164931-77-5P 164931-78-6P 174782-76-4P

RL: SPN (Synthetic preparation); PREP (Preparation)
(aluminum-BINOL complex as asym. catalyst for Michael addns.
and tandem Michael-aldol reactions)

RN 164931-77-5 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, dimethyl ester (9CI)
(CA INDEX NAME)

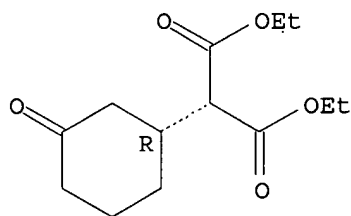
Absolute stereochemistry. Rotation (+).



RN 164931-78-6 HCAPLUS

CN Propanedioic acid, [(1R)-3-oxocyclohexyl]-, diethyl ester (9CI)
(CA INDEX NAME)

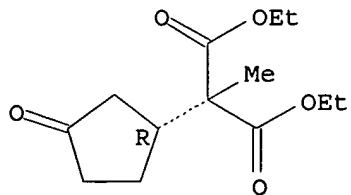
Absolute stereochemistry. Rotation (+).



RN 174782-76-4 HCAPLUS

CN Propanedioic acid, methyl[(1R)-3-oxocyclopentyl]-, diethyl ester
(9CI) (CA INDEX NAME)

Absolute stereochemistry.



CC 24-5 (Alicyclic Compounds)
Section cross-reference(s): 75

- IT Aldol condensation catalysts
Asymmetric synthesis and induction
Michael reaction catalysts
 (aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)
- IT 100-52-7, Benzaldehyde, reactions 104-53-0, 3-Phenylpropanal
 105-53-3, Diethyl malonate 108-59-8, Dimethyl malonate
 609-08-5, Diethyl methylmalonate 930-30-3,
 2-Cyclopentenone 930-68-7, 2-Cyclohexenone 15014-25-2,
 Dibenzyl malonate
 RL: RCT (Reactant); **R**ACT (Reactant or reagent)
 (aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)
- IT 164931-75-3P **164931-77-5P** **164931-78-6P**
174782-76-4P 174782-78-6P 174782-84-4P 185760-71-8P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (aluminum-BINOL complex as asym. catalyst for Michael addns. and tandem Michael-aldol reactions)

L93 ANSWER 29 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:961627 HCAPLUS

DOCUMENT NUMBER: 124:174937

TITLE: Ruthenium-catalyzed aldol and Michael reactions of nitriles. Carbon-carbon bond formation by α -C-H activation of nitriles.

AUTHOR(S): Murahashi, Shun-Ichi; Naota, Takeshi; Taki, Hiroshi; Mizuno, Masahiko; Takaya, Hikaru; Komiya, Sanshiro; Mizuho, Yuji; Oyasato, Naohiko; Hiraoka, Makiko; et al.

CORPORATE SOURCE: Faculty of Engineering Science, Osaka University, Toyonaka, 560, Japan

SOURCE: Journal of the American Chemical Society (1995), 117(50), 12436-51

CODEN: JACSAT; ISSN: 0002-7863

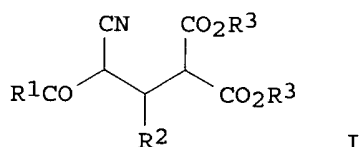
PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:174937

GI



- AB Ru(II)-catalyzed reaction of nitriles with carbonyl compds. proceeds efficiently under mild conditions to give α,β -unsatd. nitriles. Under similar reaction conditions, nitriles react with olefins bearing electron-withdrawing groups to give Michael adducts. The utility of the reaction is illustrated by selective addns. to α,β -unsatd. aldehydes and acetylenes bearing electron-withdrawing groups, which are difficult to perform using conventional bases. Chemoselective aldol and Michael reactions of nitriles can be performed in the presence of other active

methylene compds. Michael and tandem Michael-aldol condensations of nitriles (I; R1 = OMe, OEt, OBu, NH2; R2, R3 = Me, Et) with H2C:CHEWG (EWG = COMe, CN, CPh) can be performed with high diastereoselectivity. These reactions can be rationalized by assuming oxidative addition of Ru(0) to the α -C-H bond of nitriles and subsequent insertions to carbonyl compds. or olefins. As the key intermediates and active catalysts hydrido(N-bonded enolato)Ru(II) complexes, mer-RuH(NCCHCO2R)(NCCH2CO2R)(PPh3)3 (R = Me, Et, Bu) have been isolated upon treatment of RuH2(PPh3)4 or RuH(C2H4)(PPh3)2(PPh2C6H4) with alkyl cyanoacetates. Kinetic study of the catalytic aldol reaction of Et cyanoacetate with PhCHO indicates that the rate-determining step is the reaction of enolato complex with aldehydes.

ED Entered STN: 05 Dec 1995

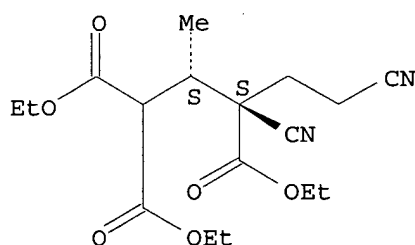
IT 173593-92-5P

RL: BYP (Byproduct); PREP (Preparation)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

RN 173593-92-5 HCAPLUS

CN 1,1,3-Pentanetricarboxylic acid, 3,5-dicyano-2-methyl-, triethyl ester, (R*,R*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.

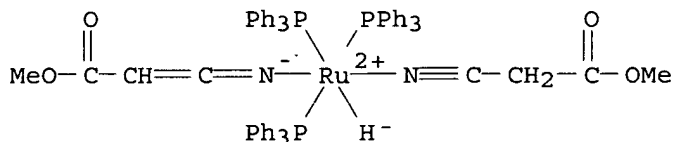


IT 138614-12-7P 138614-14-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);
PREP (Preparation); RACT (Reactant or reagent)
(ruthenium-catalyzed aldol and Michael reactions of nitriles)

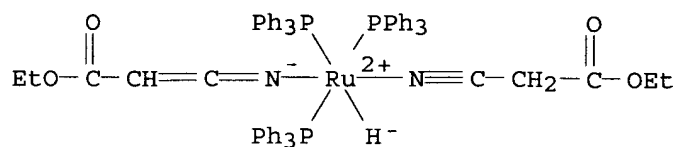
RN 138614-12-7 HCAPLUS

CN Ruthenium, hydro(methyl carbonimidoylacetato-N)(methyl cyanoacetato-N)tris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)

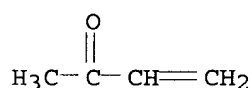


RN 138614-14-9 HCAPLUS

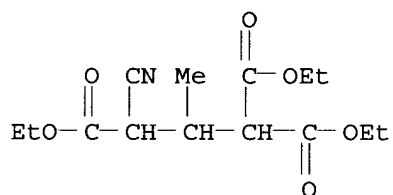
CN Ruthenium, [ethyl (cyano- κ N)acetate][ethyl 3-(imino- κ N)-2-propenoato]hydrotris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)



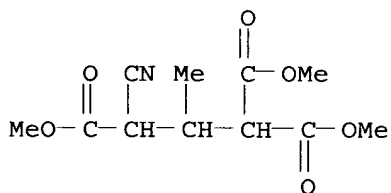
IT 78-94-4, Methyl vinyl ketone, reactions
 121730-78-7 173594-02-0 173594-03-1
 173594-04-2 173594-05-3
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (ruthenium-catalyzed aldol and Michael reactions of nitriles)
 RN 78-94-4 HCAPLUS
 CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



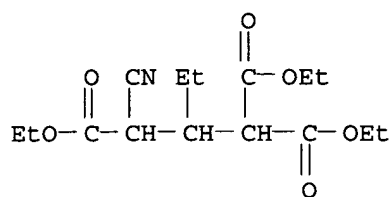
RN 121730-78-7 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl ester
 (9CI) (CA INDEX NAME)



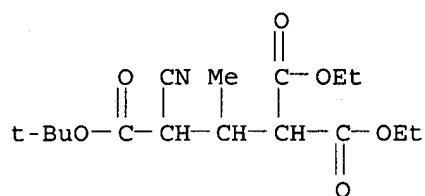
RN 173594-02-0 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, trimethyl ester (9CI) (CA INDEX NAME)



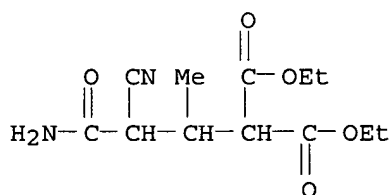
RN 173594-03-1 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-ethyl-, triethyl ester
 (9CI) (CA INDEX NAME)



RN 173594-04-2 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-,
 3-(1,1-dimethylethyl) 1,1-diethyl ester (9CI) (CA INDEX NAME)

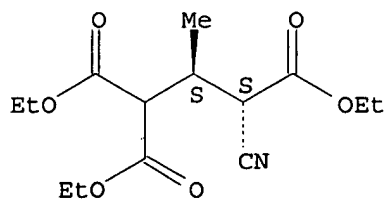


RN 173594-05-3 HCAPLUS
 CN Propanedioic acid, (3-amino-2-cyano-1-methyl-3-oxopropyl)-,
 diethyl ester (9CI) (CA INDEX NAME)



IT 173593-73-2P 173593-75-4P 173593-87-8P
 173593-97-0P 173594-00-8P 173594-01-9P
 173828-21-2P 173828-22-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (ruthenium-catalyzed aldol and Michael reactions of nitriles)
 RN 173593-73-2 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl
 ester, (R*,R*)- (9CI) (CA INDEX NAME)

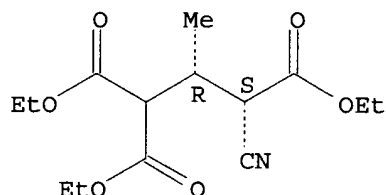
Relative stereochemistry.



RN 173593-75-4 HCAPLUS
 CN 1,1,3-Propanetricarboxylic acid, 3-cyano-2-methyl-, triethyl

ester, (R*,S*)- (9CI) (CA INDEX NAME)

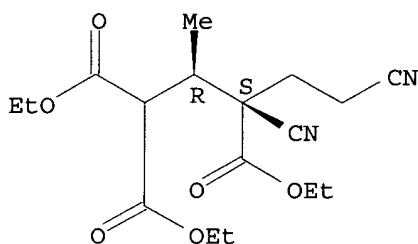
Relative stereochemistry.



RN 173593-87-8 HCAPLUS

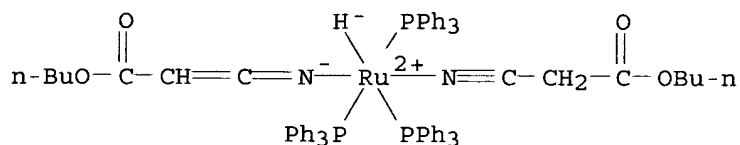
CN 1,1,3-Pentanetricarboxylic acid, 3,5-dicyano-2-methyl-, triethyl ester, (R*,S*)- (9CI) (CA INDEX NAME)

Relative stereochemistry.



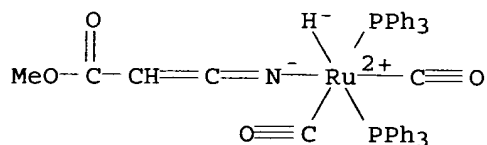
RN 173593-97-0 HCAPLUS

CN Ruthenium, (butyl cyanoacetate-N)(butyl 3-imino-2-propenoato-N)hydrotris(triphenylphosphine)-, (OC-6-31)- (9CI) (CA INDEX NAME)



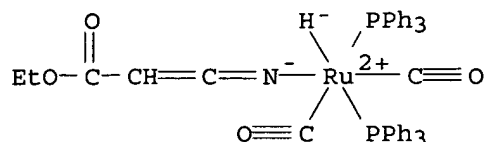
RN 173594-00-8 HCAPLUS

CN Ruthenium, dicarbonylhydro(methyl 3-imino-2-propenoato-N)bis(triphenylphosphine)-, (OC-6-13)- (9CI) (CA INDEX NAME)



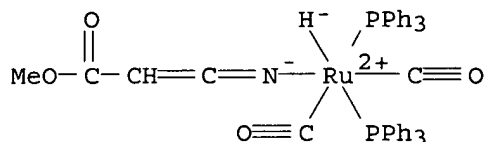
RN 173594-01-9 HCAPLUS

CN Ruthenium, dicarbonyl(ethyl 3-imino-2-propenoato-N)hydrobis(triphenylphosphine)-, (OC-6-13)- (9CI) (CA INDEX NAME)



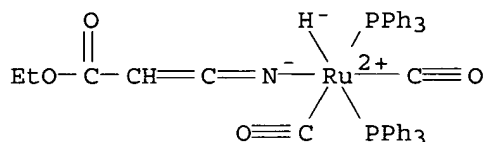
RN 173828-21-2 HCAPLUS

CN Ruthenium, dicarbonylhydro(methyl 3-imino-2-propenoato-N)bis(triphenylphosphine)-, (OC-6-14)- (9CI) (CA INDEX NAME)



RN 173828-22-3 HCAPLUS

CN Ruthenium, dicarbonyl(ethyl 3-imino-2-propenoato-N)hydrobis(triphenylphosphine)-, (OC-6-14)- (9CI) (CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 22

IT Aldol condensation

Aldol condensation catalysts

Michael reaction

Michael reaction catalysts

Quantitative structure-activity relationship

(ruthenium-catalyzed aldol and Michael reactions of nitriles)

IT 121787-49-3P 173593-92-5P 173593-93-6P

RL: BYP (Byproduct); PREP (Preparation)

(ruthenium-catalyzed aldol and Michael reactions of nitriles)

IT 138614-12-7P 138614-14-9P

RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation);

PREP (Preparation); RACT (Reactant or reagent)

(ruthenium-catalyzed aldol and Michael reactions of nitriles)

IT 74-88-4, Methyl iodide, reactions 78-94-4, Methyl vinyl

ketone, reactions 79-24-3, Nitroethane 96-33-3 100-50-5,

3-Cyclohexene-1-carboxaldehyde 100-52-7, Benzaldehyde, reactions

105-45-3, Methyl acetoacetate 105-56-6, Ethyl cyanoacetate

107-02-8, Acrolein, reactions 107-13-1, 2-Propenenitrile,

reactions 108-59-8, Dimethyl malonate 108-94-1, Cyclohexanone,

reactions 109-77-3, Dicyanomethane 123-08-0,

4-Hydroxybenzaldehyde 123-11-5, 4-Methoxybenzaldehyde, reactions

123-54-6, 2,4-Pentanedione, reactions 123-72-8, Butyraldehyde

140-29-4, Benzyl cyanide 140-88-5 495-41-0 538-51-2,

N-Benzylideneaniline 623-47-2, Ethyl propiolate 627-26-9

630-08-0, Carbon monoxide, reactions 768-03-6, Phenyl vinyl

ketone 1190-76-7 1423-60-5, Ethynyl methyl ketone 1462-12-0,

Diethyl ethylidenemalonate 1572-99-2, Ethyl 2-cyanopropionate

1823-91-2, 2-Phenylpropionitrile 3696-36-4 5459-58-5, Butyl
cyanoacetate 5832-70-2 17085-88-0, Diethyl propylidenemalonate
59853-02-0 121730-78-7 173594-02-0

173594-03-1 173594-04-2 173594-05-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(ruthenium-catalyzed aldol and Michael reactions of nitriles)

IT 921-75-5P 1112-27-2P 2017-87-0P 2169-69-9P 4335-90-4P
4354-73-8P, Cyclohexylidenemalononitrile 6802-76-2P
14533-86-9P 14618-77-0P, Methyl 2-cyanopropanoate 15709-57-6P
30378-23-5P, Ethyl 2,4-dicyano-2-methylbutanoate 42205-38-9P
51067-99-3P 57812-20-1P 58774-06-4P 102746-75-8P,
2-Methyl-2-phenylpentanedinitrile 118745-25-8P, Ethyl
(E)-2-cyano-2-hexenoate 118745-26-9P 118745-27-0P
121754-82-3P 155696-60-9P 173593-73-2P 173593-74-3P
173593-75-4P 173593-76-5P 173593-77-6P 173593-78-7P
173593-79-8P 173593-80-1P 173593-81-2P 173593-82-3P
173593-83-4P 173593-84-5P 173593-85-6P 173593-87-8P
173593-88-9P 173593-89-0P 173593-91-4P 173593-94-7P
173593-95-8P 173593-96-9P 173593-97-0P 173593-98-1P
173593-99-2P 173594-00-8P 173594-01-9P
173594-06-4P 173594-07-5P 173828-19-8P 173828-20-1P
173828-21-2P 173828-22-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(ruthenium-catalyzed aldol and Michael reactions of nitriles)

L93 ANSWER 30 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1995:938755 HCAPLUS

DOCUMENT NUMBER: 124:55338

TITLE: Catalytic activity of polymerizable metal
 β -ketoesterato complexes towards Michael
addition reactions

AUTHOR(S): Mastroilli, P.; Nobile, C. F.; Suranna, G. P.

CORPORATE SOURCE: Centro di studi CNR sulle Metodologie
Innovative in Sintesi Organiche M.I.S.O.,
Istituto di Chimica del Politecnico di Bari,
trav. 200 Re David 4, Bari, I-70126, Italy

SOURCE: Journal of Molecular Catalysis A: Chemical (1995), 103(1), 23-9

CODEN: JMCCF2; ISSN: 1381-1169

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 124:55338

AB The addition of β -dioxo compds. $R1C(O)CH_2C(O)R_2$ ($R_1 = R_2 = Me$ or
OEt, $R_1 = Me$, $R_2 = OMe$) to Me vinyl ketone was catalyzed by Ni(II)
and Co(II) complexes with the polymerizable β -ketoesterato
2-(acetoacetoxy)ethyl methacrylate (AAEMA-) under homogeneous and
heterogeneous phases to give $R1C(O)CH[C(O)R_2]CH_2CH_2C(O)Me$. The
homogeneous reactions were carried out using the soluble Ni(AAEMA)₂
and Co(AAEMA)₂ complexes whereas the heterogeneous catalytic tests
were carried out using the copolymers obtained by reaction of
M(AAEMA)₂ (M = Ni or Co) with suitable acrylamides. The Co(II)
catalysts were more active than the Ni(II) catalysts in both the
homogeneous and heterogeneous phases.

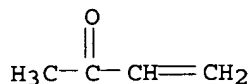
ED Entered STN: 23 Nov 1995

IT 78-94-4, Methyl vinyl ketone, reactions

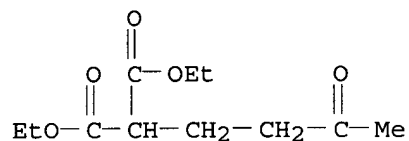
RL: RCT (Reactant); RACT (Reactant or reagent)

(Michael addition of β -dioxo compds. with Me vinyl ketone
catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate
complexes and their acrylamide copolymers)

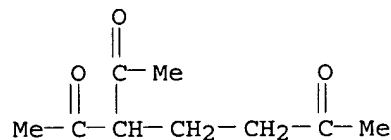
RN 78-94-4 HCAPLUS
 CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



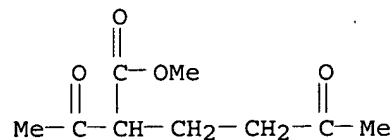
IT 4761-26-6P 29214-57-1P, 3-Acetylheptane-2,6-dione 35490-04-1P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (Michael addition of β -dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxy)ethyl methacrylate complexes and their acrylamide copolymers)
 RN 4761-26-6 HCAPLUS
 CN Propanedioic acid, (3-oxobutyl)-, diethyl ester (9CI) (CA INDEX NAME)



RN 29214-57-1 HCAPLUS
 CN 2,6-Heptanedione, 3-acetyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 35490-04-1 HCAPLUS
 CN Hexanoic acid, 2-acetyl-5-oxo-, methyl ester (9CI) (CA INDEX NAME)



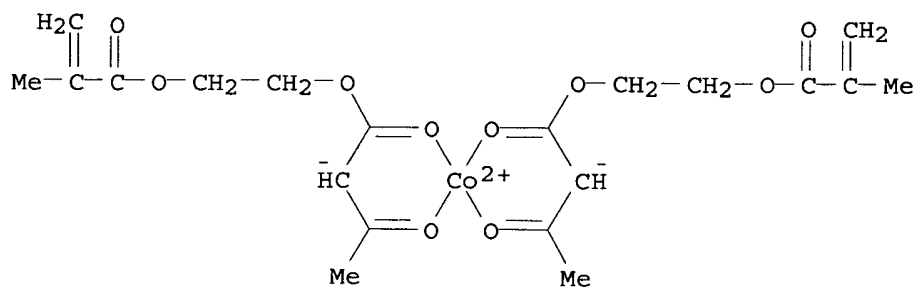
IT 172172-22-4P 172172-23-5P
 RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
 (preparation as catalyst for Michael addition of β -dioxo compds. with Me vinyl ketone)
 RN 172172-22-4 HCAPLUS
 CN Cobalt, bis[[(2-methyl-1-oxo-2-propenyl)oxy]ethyl 3-(oxo- κ O)butanoato- κ O']-, polymer with N,N'-dimethyl-2-propenamide and N,N'-methylenabis[2-propenamide] (9CI) (CA INDEX NAME)

CM 1

CRN 156127-94-5

CMF C20 H26 Co O10

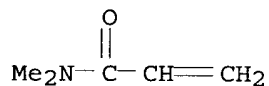
CCI CCS



CM 2

CRN 2680-03-7

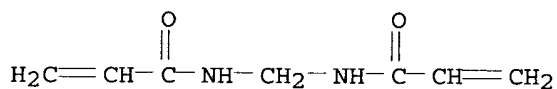
CMF C5 H9 N O



CM 3

CRN 110-26-9

CMF C7 H10 N2 O2



RN 172172-23-5 HCAPLUS

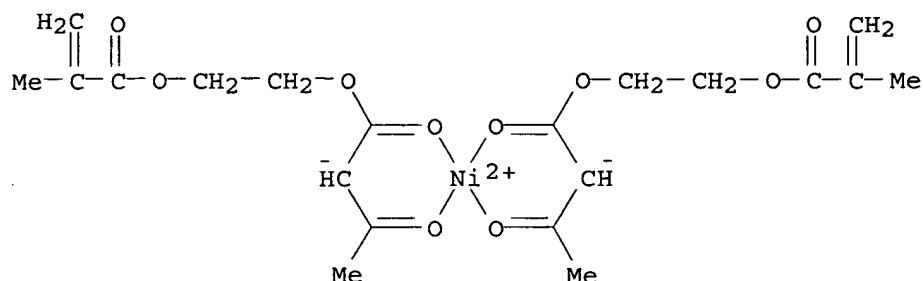
CN Nickel, bis[[(2-methyl-1-oxo-2-propenyl)oxy]ethyl
3-oxobutanoato-O1,O3]-, polymer with N,N-dimethyl-2-propenamide
and N,N'-methylenebis[2-propenamide] (9CI) (CA INDEX NAME)

CM 1

CRN 156127-92-3

CMF C20 H26 Ni O10

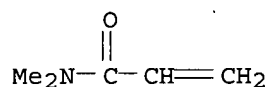
CCI CCS



CM 2

CRN 2680-03-7

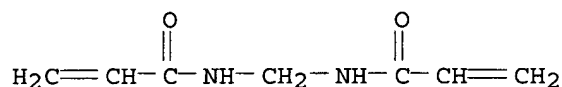
CMF C5 H9 N O



CM 3

CRN 110-26-9

CMF C7 H10 N2 O2

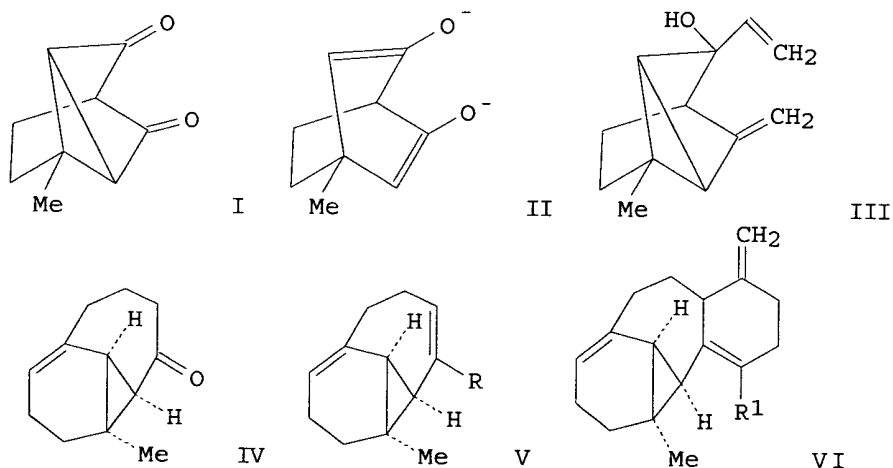


CC 23-17 (Aliphatic Compounds)
Section cross-reference(s): 35, 67

- IT **Michael reaction catalysts**
(nickel and cobalt (acetoacetoxyl)ethyl methacrylate complexes and their acrylamide copolymers for β -dioxo compds. with Me vinyl ketone)
- IT **78-94-4**, Methyl vinyl ketone, reactions 105-45-3, Methyl acetoacetate 105-53-3, Diethyl malonate 123-54-6, 2,4-Pentanedione, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(Michael addition of β -dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxyl)ethyl methacrylate complexes and their acrylamide copolymers)
- IT **4761-26-6P 29214-57-1P**, 3-Acetylheptane-2,6-dione **35490-04-1P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(Michael addition of β -dioxo compds. with Me vinyl ketone catalyzed by nickel and cobalt (acetoacetoxyl)ethyl methacrylate complexes and their acrylamide copolymers)
- IT **172172-22-4P 172172-23-5P**
RL: CAT (Catalyst use); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(preparation as catalyst for Michael addition of β -dioxo compds.)

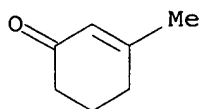
with Me vinyl ketone)

L93 ANSWER 31 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1993:581045 HCAPLUS
 DOCUMENT NUMBER: 119:181045
 TITLE: Studies directed toward the total synthesis of
 cerorubenic acid-III. 1. Expedient
 construction of the tetracyclic core by
 oxyanionic sigmatropy
 AUTHOR(S): Paquette, Leo A.; Poupart, Marc Andre
 CORPORATE SOURCE: Evans Chem. Lab., Ohio State Univ., Columbus,
 OH, 43210, USA
 SOURCE: Journal of Organic Chemistry (1993),
 58(16), 4245-53
 CODEN: JOCEAH; ISSN: 0022-3263
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 119:181045
 GI

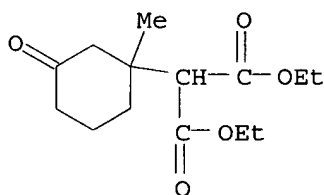


AB A synthesis of the ABCD ring framework of cerorubenic acid-III is described. Diketone I was first prepared by intramol. oxidative coupling of the dienolate II and then suitably desymmetrized to deliver III. Anionic oxy-Cope rearrangement of this intermediate resulted in construction of IV, a ketone not only having all three contiguous stereogenic centers properly established but also equipped with adequate functionality for the further elaboration of ring D. In the present effort, this thrust took the form of homologation to V (R = Ac), conversion to the activated diene V [R = C(OSiMe₂CMe₃):CH₂], and Diels-Alder cycloaddn. to Me acrylate at high pressure. Once it became obvious that first-formed ketone greatly preferred adoption of trans stereochem. at the ring juncture, attempts to skirt this issue were made by preparing both VI (R1 = CN) and VI (R1 = Ac). However, these advanced intermediates proved unresponsive to conjugate reduction, and attention was therefore redirected to alternative possible means for elaboration of the eastern sector.

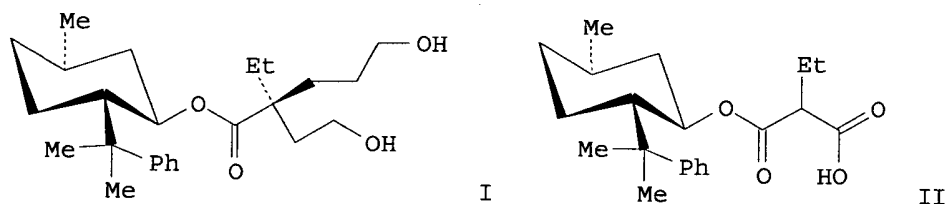
ED Entered STN: 30 Oct 1993
 IT 1193-18-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conjugate vinylation or Michael addition to, by malonate)
 RN 1193-18-6 HCAPLUS
 CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



IT 88710-73-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation, saponification, and decarboxylation of)
 RN 88710-73-0 HCAPLUS
 CN Propanedioic acid, (1-methyl-3-oxocyclohexyl)-, diethyl ester
 (9CI) (CA INDEX NAME)



CC 30-25 (Terpenes and Terpenoids)
 IT Asymmetric synthesis and induction
 (of cerorubenic acid-III tetracyclic core)
 IT 1193-18-6
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (conjugate vinylation or Michael addition to, by malonate)
 IT 88710-73-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP
 (Preparation); RACT (Reactant or reagent)
 (preparation, saponification, and decarboxylation of)
 L93 ANSWER 32 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 1992:571787 HCAPLUS
 DOCUMENT NUMBER: 117:171787
 TITLE: Enantioselective construction of a quaternary
 stereogenic center via tandem acid anhydride
 formation-intramolecular Michael reaction
 AUTHOR(S): Ihara, Masataka; Taniguchi, Nobuaki; Suzuki,
 Shuichi; Fukumoto, Keiichiro
 CORPORATE SOURCE: Pharm. Inst., Tohoku Univ., Sendai, 980, Japan
 SOURCE: Journal of the Chemical Society, Chemical
 Communications (1992), (14), 976-7
 CODEN: JCCCCAT; ISSN: 0022-4936
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 OTHER SOURCE(S): CASREACT 117:171787
 GI



AB A novel method for the enantioselective construction of a quaternary stereogenic center by tandem acid anhydride formation-intramol. Michael reaction has been developed; a synthetic intermediate I for Hunteria and Aspidosperma indole alkaloids has been prepared by the application of this procedure using acid II and acryloyl chloride.

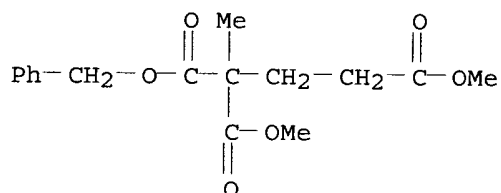
ED Entered STN: 01 Nov 1992

IT **143723-43-7P**

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 143723-43-7 HCAPLUS

CN 1,3,3-Butanetricarboxylic acid, 1,3-dimethyl 3-(phenylmethyl)
ester (9CI) (CA INDEX NAME)

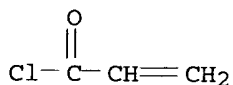


IT **814-68-6**, Acryloyl chloride

RL: RCT (Reactant); **RACT (Reactant or reagent)**
(reaction of, with chiral half ester and subsequent intramol.
Michael reaction)

RN 814-68-6 HCAPLUS

CN 2-Propenoyl chloride (9CI) (CA INDEX NAME)



CC 31-5 (Alkaloids)

Section cross-reference(s): 22

IT **Asymmetric synthesis and induction**

(in tandem acid anhydride formation-intramol. Michael reaction)

IT **Michael reaction**

(intramol., tandem acid anhydride formation and, in synthesis
of indole alkaloid intermediate)

IT 123463-89-8P 132143-23-8P **143723-43-7P** 143723-44-8P

143723-45-9P 143723-48-2P 143723-50-6P 143723-53-9P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

IT **814-68-6**, Acryloyl chloride

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with chiral half ester and subsequent intramol.
 Michael reaction)

L93 ANSWER 33 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1991:142264 HCAPLUS

DOCUMENT NUMBER: 114:142264

TITLE: Michael addition promoted by bis-bidentate
 nickel(II) Schiff base complexes derived from
 aromatic 2-hydroxy aldehydes

AUTHOR(S): Botteghi, C.; Schionato, A.; Rosini, C.;
 Salvadori, P.

CORPORATE SOURCE: Dip. Chim., Univ. Venezia, Venice, 30123,
 Italy

SOURCE: Journal of Molecular Catalysis (1990
), 63(2), 155-65

CODEN: JMCADS; ISSN: 0304-5102

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 114:142264

AB Bis-bidentate Ni(II) Schiff-base complexes derived from
 2-HOC6H4CHO or hydroxynaphthaldehydes catalyze the Michael addition
 of β -oxo esters to MeCOCH:CH₂. Complexes with prevailing
 square-planar structure in solution are more active than their
 tetrahedral isomers. Low optical inductions ($\leq 6\%$) are
 observed only if the Michael addns. are carried out in the presence
 of square-planar complexes with optically active Schiff-base
 ligands.

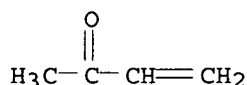
ED Entered STN: 19 Apr 1991

IT 78-94-4, Methyl vinyl ketone, reactions 930-68-7
 , 2-Cyclohexen-1-one

RL: RCT (Reactant); RACT (Reactant or reagent)
 (Michael addition reaction of, with dicarbonyl compds., catalysts
 for)

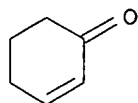
RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



RN 930-68-7 HCAPLUS

CN 2-Cyclohexen-1-one (6CI, 8CI, 9CI) (CA INDEX NAME)



IT 14322-02-2 15379-94-9 15390-05-3

56647-29-1 56647-30-4

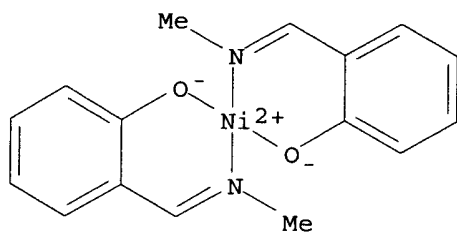
RL: CAT (Catalyst use); USES (Uses)

(catalyst, for Michael addition reaction of dicarbonyl compds.
 with unsatd. ketones)

RN 14322-02-2 HCAPLUS

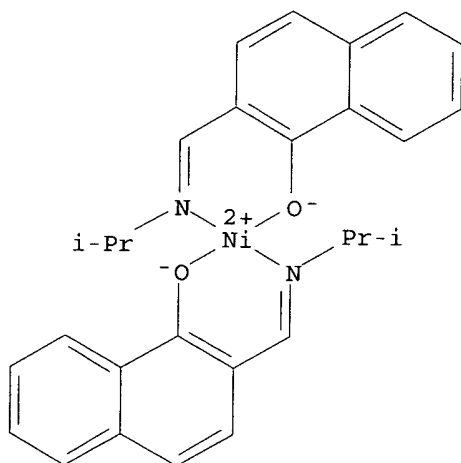
CN Nickel, bis[2-[(methylimino- κ N)methyl]phenolato- κ O]-

(9CI) (CA INDEX NAME)



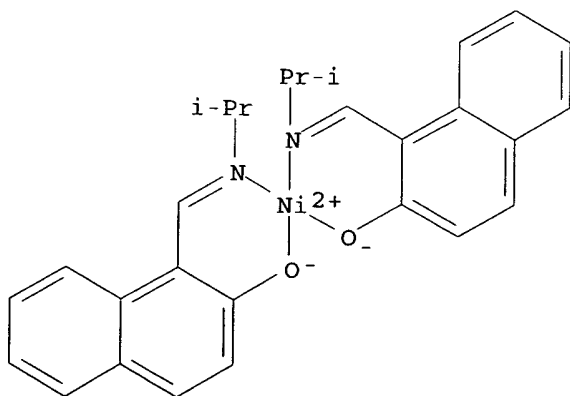
RN 15379-94-9 HCAPLUS

CN Nickel, bis[2-[[1-methylethyl]imino]methyl]-1-naphthalenolato-N,O]- (9CI) (CA INDEX NAME)



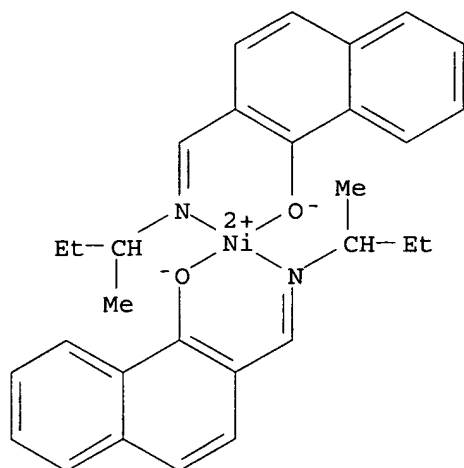
RN 15390-05-3 HCAPLUS

CN Nickel, bis[1-[[1-methylethyl]imino]methyl]-2-naphthalenolato-N,O]- (9CI) (CA INDEX NAME)

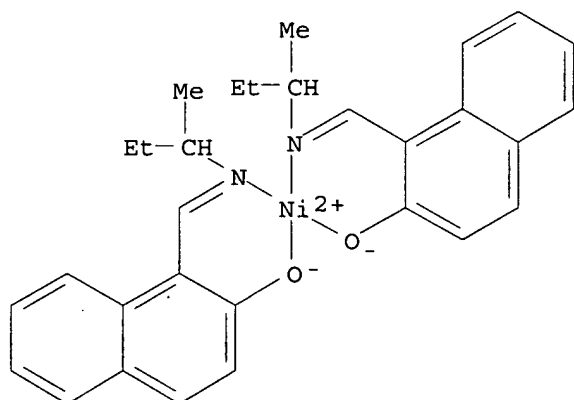


RN 56647-29-1 HCAPLUS

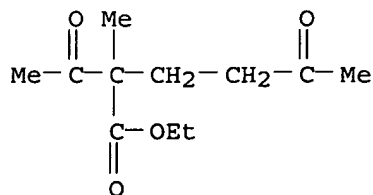
CN Nickel, bis[2-[[1-methylpropyl]imino]methyl]-1-naphthalenolato-N,O]- (9CI) (CA INDEX NAME)



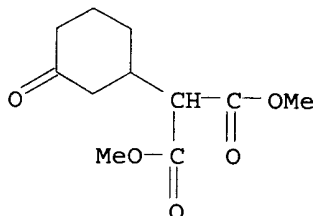
RN 56647-30-4 HCAPLUS
 CN Nickel, bis[1-[[[(1-methylpropyl)imino]methyl]-2-naphthalenolato-
 N,O]-, [SP-4-1-(S),(S)]- (9CI) (CA INDEX NAME)



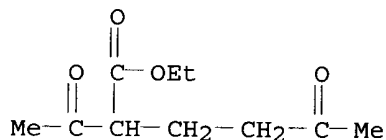
IT 28793-08-0P 33646-18-3P 35490-05-2P
 66152-63-4P 78044-62-9P 94410-52-3P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
 RN 28793-08-0 HCAPLUS
 CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester (6CI, 8CI,
 9CI) (CA INDEX NAME)



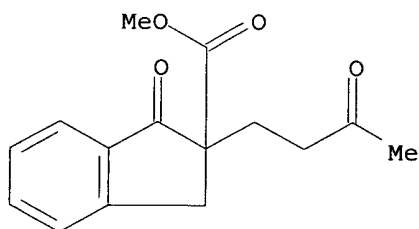
RN 33646-18-3 HCAPLUS
 CN Propanedioic acid, (3-oxocyclohexyl)-, dimethyl ester (9CI) (CA INDEX NAME)



RN 35490-05-2 HCAPLUS
 CN Hexanoic acid, 2-acetyl-5-oxo-, ethyl ester (6CI, 7CI, 9CI) (CA INDEX NAME)

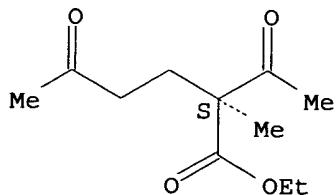


RN 66152-63-4 HCAPLUS
 CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-, methyl ester (9CI) (CA INDEX NAME)



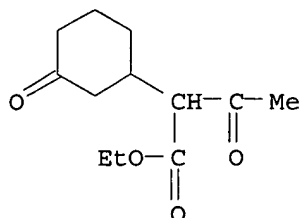
RN 78044-62-9 HCAPLUS
 CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).



RN 94410-52-3 HCAPLUS
 CN Cyclohexaneacetic acid, α-acetyl-3-oxo-, ethyl ester (9CI)

(CA INDEX NAME)



CC 21-2 (General Organic Chemistry)

Section cross-reference(s): 25

IT **Michael reaction catalysts**

(nickel complexes of Schiff bases derived from aromatic hydroxy aldehydes, for dicarbonyl compds. with unsatd. ketones)

IT **Michael reaction**

(of dicarbonyl compds. with unsatd. ketones, catalytic)

IT 78-94-4, Methyl vinyl ketone, reactions 930-68-7

, 2-Cyclohexen-1-one

RL: RCT (Reactant); RACT (Reactant or reagent)

(Michael addition reaction of, with dicarbonyl compds., catalysts for)

IT 14322-02-2 15379-94-9 15390-05-3

56647-29-1 56647-30-4

RL: CAT (Catalyst use); USES (Uses)

(catalyst, for Michael addition reaction of dicarbonyl compds. with unsatd. ketones)

IT 28793-08-0P 33646-18-3P 35490-05-2P

66152-63-4P 78044-62-9P 94410-52-3P

132931-89-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

L93 ANSWER 34 OF 34 HCAPLUS COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 1984:209326 HCAPLUS

DOCUMENT NUMBER: 100:209326

TITLE: Asymmetric catalyses. Part 18.
Enantioselective Michael additions using
optically active cobalt(II)/diamine catalysts

AUTHOR(S): Brunner, Henri; Hammer, Benedikt

CORPORATE SOURCE: Inst. Anorg. Chem., Univ. Regensburg,

Regensburg, D-8400, Fed. Rep. Ger.

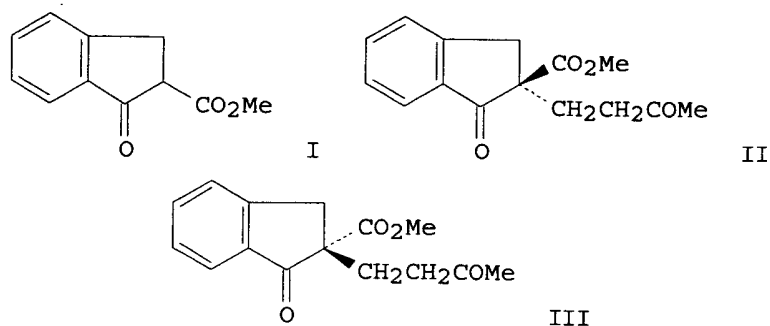
SOURCE: Angewandte Chemie (1984), 96(4),
305-6

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal

LANGUAGE: German

GI



AB Co(acac)₂(nn) [acac = MeCOCH₂COMe, nn = (+)- or (-)-H₂NCHPhCHPhNH₂] catalyzed the enantioselective Michael addition of H₂C:CHCOMe to indancarboxylate I to give the addition product II or III in enantiomeric excess (ee). H₂C:CHCOMe added to I in 40 h at 20° with Co(acac)₂[(+)-nn] to give 79% yield of II with 21.3% ee. This ee yield increased with decreasing temperature to 66% ee at -50° in 64 h. (-)-(Nn) gave 5.8% ee of II at 20° but Co(acac)₂[(-)-nn] gave 37.2 and 58.3% ee of III at -20 and -40°, resp. H₂C:CHCOMe and MeCOCHMeCO₂Et under Co(acac)₂[(+)-nn] catalysis gave 4.5% ee of Michael adduct at room temperature

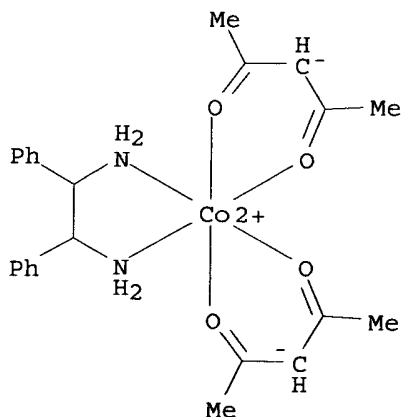
ED Entered STN: 23 Jun 1984

IT 89485-98-3

RL: CAT (Catalyst use); USES (Uses)
(catalyst, for enantioselective Michael addition of indancarboxylate with 1,3-dicarbonyl compds.)

RN 89485-98-3 HCAPLUS

CN Cobalt, (1,2-diphenyl-1,2-ethanediamine-N,N')bis(2,4-pentanedionato-O,O')-, [OC-6-21-[S-(R*,R*)]]- (9CI) (CA INDEX NAME)

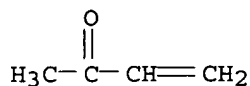


IT 78-94-4, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)
(enantioselective Michael addition reaction of, with indancarboxylate in presence of cobalt(II)-optically active diamines)

RN 78-94-4 HCAPLUS

CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



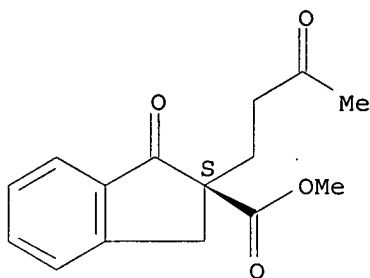
IT 58623-84-0P 78044-62-9P 79298-08-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 58623-84-0 HCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-,
methyl ester, (2S)- (9CI) (CA INDEX NAME)

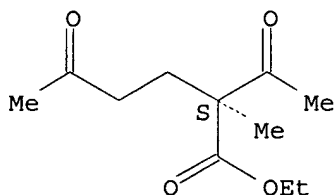
Absolute stereochemistry. Rotation (-).



RN 78044-62-9 HCAPLUS

CN Hexanoic acid, 2-acetyl-2-methyl-5-oxo-, ethyl ester, (2S)- (9CI)
(CA INDEX NAME)

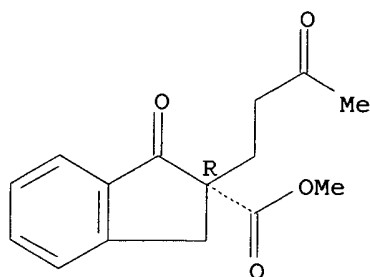
Absolute stereochemistry. Rotation (-).



RN 79298-08-1 HCAPLUS

CN 1H-Indene-2-carboxylic acid, 2,3-dihydro-1-oxo-2-(3-oxobutyl)-,
methyl ester, (2R)- (9CI) (CA INDEX NAME)

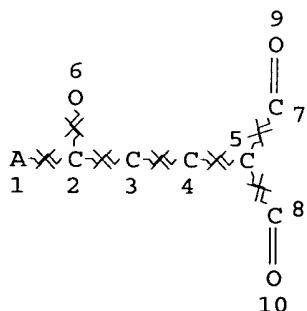
Absolute stereochemistry. Rotation (+).



- CC 25-23 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
 Section cross-reference(s): 22
- IT **Asymmetric synthesis and induction**
 (Michael adducts, of indancarboxylates with 1,3-dicarbonyl compds. in presence of cobalt(II)-optically active diamine catalysts)
- IT **Michael reaction catalysts**
 (cobalt(II)-optically active diamines, for indancarboxylates with 1,3-dicarbonyl compds.)
- IT **Michael reaction**
 (enantioselective, of indancarboxylates with 1,3-dicarbonyl compds.)
- IT **89485-98-3**
 RL: CAT (Catalyst use); USES (Uses)
 (catalyst, for enantioselective Michael addition of indancarboxylate with 1,3-dicarbonyl compds.)
- IT **78-94-4, reactions 609-14-3**
 RL: RCT (Reactant); **RACT (Reactant or reagent)**
 (enantioselective Michael addition reaction of, with indancarboxylate in presence of cobalt(II)-optically active diamines)
- IT **58623-84-0P 78044-62-9P 79298-08-1P**
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

=> => d que 1111

L21 SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010
 L25 STR



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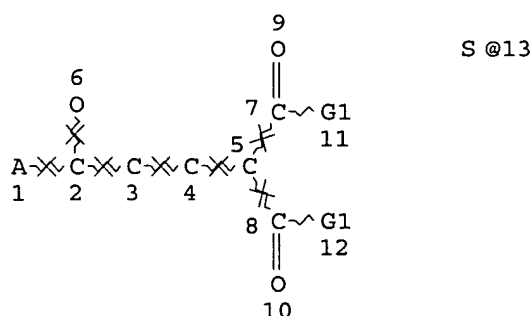
CONNECT IS X2 RC AT 6
 CONNECT IS E1 RC AT 9
 CONNECT IS E1 RC AT 10

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DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 10

STEREO ATTRIBUTES: NONE

L27 12118 SEA FILE=REGISTRY SSS FUL L25 NOT L21
L30 STR



VAR G1=O/N/P/13

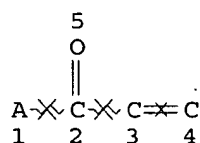
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CONNECT IS X2 RC AT 6
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L32 2503 SEA FILE=REGISTRY SUB=L27 SSS FUL L30
L37 STR



NODE ATTRIBUTES:

CONNECT IS E1 RC AT 5
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 5

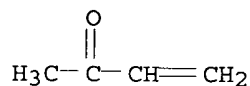
STEREO ATTRIBUTES: NONE

L40 SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005
L42 6815 SEA FILE=REGISTRY SSS FUL L37 NOT L40
L106 816 SEA FILE=CAOLD ABB=ON PLU=ON L27
L107 175 SEA FILE=CAOLD ABB=ON PLU=ON L32

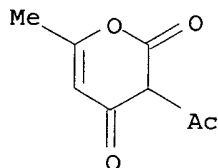
L108 1649 SEA FILE=CAOLD ABB=ON PLU=ON L42
 L109 21 SEA FILE=CAOLD ABB=ON PLU=ON L106 AND L108
 L110 6 SEA FILE=CAOLD ABB=ON PLU=ON L108 AND L107
 L111 21 SEA FILE=CAOLD ABB=ON PLU=ON L109 OR L110

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L111 ANSWER 1 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: CA63:8636c CAOLD
 TITLE: tryptophan metabolism
 AUTHOR NAME: Scott, Thomas Arthur
 INDEX TERM: 57-57-8 67-47-0 78-94-4
 108-30-5 128-53-0 151-56-4 498-23-7
 520-45-6 551-16-6 616-02-4 768-03-6
 872-36-6 2170-03-8
 IT 78-94-4 520-45-6
 RN 78-94-4 CAOLD
 CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



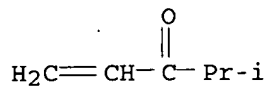
RN 520-45-6 CAOLD
 CN 2H-Pyran-2,4(3H)-dione, 3-acetyl-6-methyl- (8CI, 9CI) (CA INDEX NAME)



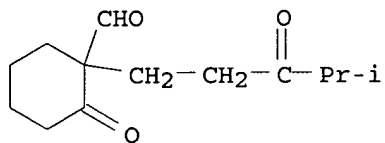
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 128-53-0 151-56-4 498-23-7 520-45-6 551-16-6
 616-02-4 768-03-6 872-36-6 2170-03-8

L111 ANSWER 2 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: CA62:16042e CAOLD
 TITLE: expts. in the synthesis of structure related to ring A of the triterpenes
 AUTHOR NAME: Baisted, Derek J.; Whitehurst, J. S.
 INDEX TERM: 1216-53-1 1606-24-2 1606-25-3 1606-26-4
 1606-27-5 1606-45-7 1606-47-9
 1609-24-1 1609-25-2 1839-40-3 1839-41-4
 1839-42-5 1944-81-6 1944-82-7
 2020-06-6 2020-07-7 2020-08-8 2020-09-9
 2020-10-2 2020-11-3 2020-12-4
 2020-13-5 2020-14-6 2020-15-7
 2020-16-8 2020-17-9 2020-18-0 2020-21-5
 2092-35-5 2092-36-6 2278-89-9
 2390-14-9 2420-83-9 3333-39-9 3425-62-5
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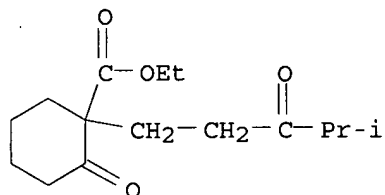
3425-71-6 3505-66-6 3758-40-5 4006-21-7
 93997-67-2 96168-60-4 98763-68-9
 99871-63-3 100658-59-1
 IT 1606-47-9 1944-81-6 2020-12-4
 2020-14-6 2092-35-5 98763-68-9
 RN 1606-47-9 CAOLD
 CN 1-Penten-3-one, 4-methyl- (8CI, 9CI) (CA INDEX NAME)



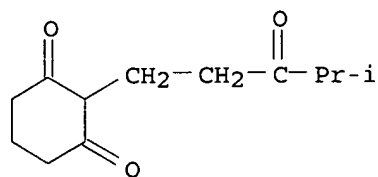
RN 1944-81-6 CAOLD
 CN Cyclohexanecarboxaldehyde, 1-(4-methyl-3-oxopentyl)-2-oxo- (7CI, 8CI) (CA INDEX NAME)



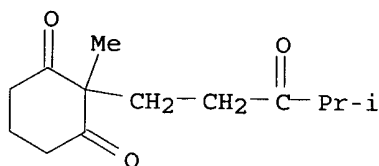
RN 2020-12-4 CAOLD
 CN Cyclohexanecarboxylic acid, 1-(4-methyl-3-oxopentyl)-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



RN 2020-14-6 CAOLD
 CN 1,3-Cyclohexanedione, 2-(4-methyl-3-oxopentyl)- (7CI, 8CI) (CA INDEX NAME)



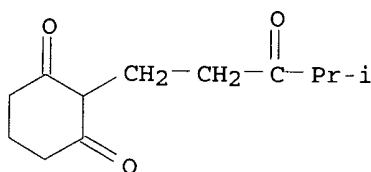
RN 2092-35-5 CAOLD
 CN 1,3-Cyclohexanedione, 2-methyl-2-(4-methyl-3-oxopentyl)- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 98763-68-9 CAOLD
 CN 1,3-Cyclohexanedione, 2-(4-methyl-3-oxopentyl)-,
 (2,4-dinitrophenyl)hydrazone (7CI) (CA INDEX NAME)

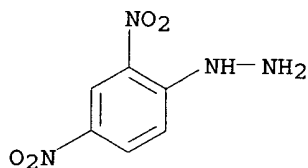
CM 1

CRN 2020-14-6
 CMF C12 H18 O3



CM 2

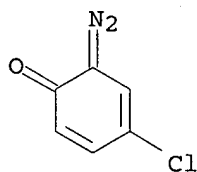
CRN 119-26-6
 CMF C6 H6 N4 O4



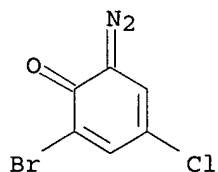
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	1606-26-4	1606-27-5	1606-45-7		
	1606-47-9	1609-24-1	1609-25-2	1839-40-3	1839-41-4
	1839-42-5	1944-81-6	1944-82-7	2020-06-6	2020-07-7
	2020-08-8	2020-09-9	2020-10-2	2020-11-3	2020-12-4
	2020-13-5	2020-14-6	2020-15-7	2020-16-8	2020-17-9
	2020-18-0	2020-21-5	2092-35-5	2092-36-6	2278-89-9
	2390-14-9	2420-83-9	3333-39-9	3425-62-5	3425-63-6
	3425-64-7	3425-65-8	3425-66-9	3425-67-0	3425-68-1
	3425-69-2	3425-70-5	3425-71-6	3505-66-6	3758-40-5
	4006-21-7	93997-67-2	96168-60-4	98763-68-9	99871-63-3
	100658-59-1				

L111 ANSWER 3 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: CA62:7903d CAOLD
 TITLE: reactions with diazocarbonyl compds. - (XIV)
 o-quinone triaminophosphazines
 AUTHOR NAME: Ried, Walter; Appel. H.

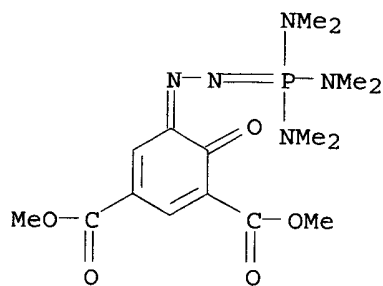
INDEX TERM: 1201-33-8 3028-26-0 3028-27-1
3028-29-3 3028-30-6 3028-31-7
3028-32-8 3028-33-9 3028-34-0 3028-35-1
3028-36-2 3028-37-3 3028-38-4 3028-39-5
3028-40-8 3028-41-9 3028-42-0 3028-43-1
3028-44-2 3028-45-3 3028-46-4
3028-47-5 3028-48-6 3028-49-7 3028-50-0
3028-51-1 3028-52-2 3028-53-3 3028-54-4
3028-55-5 3028-56-6 3028-57-7 3028-58-8
3028-59-9 3028-60-2 3028-63-5 3028-64-6
3028-65-7 3028-66-8 3028-67-9 3028-68-0
3028-69-1 3028-70-4 3028-71-5 3028-72-6
3028-73-7 3061-79-8 3065-35-8 3065-36-9
3089-74-5 3089-80-3 3089-81-4 3089-82-5
3374-09-2 3374-10-5 3441-66-5 3441-76-7
3441-77-8 3441-78-9 3441-79-0 3442-16-8
3577-41-1 3577-42-2 3978-36-7
IT 3028-27-1 3028-30-6 3028-45-3
RN 3028-27-1 CAOLD
CN 2,4-Cyclohexadien-1-one, 4-chloro-6-diazo- (6CI, 7CI, 8CI, 9CI)
(CA INDEX NAME)



RN 3028-30-6 CAOLD
CN 2,4-Cyclohexadien-1-one, 2-bromo-4-chloro-6-diazo- (7CI, 8CI) (CA
INDEX NAME)



RN 3028-45-3 CAOLD
CN Phosphorane, [(3,5-dicarboxy-6-oxo-2,4-cyclohexadien-1-ylidene)hydrazono]tris(dimethylamino)-, dimethyl ester (7CI, 8CI)
(CA INDEX NAME)



IT	1201-33-8	3028-26-0	3028-27-1		
	3028-29-3	3028-30-6	3028-31-7	3028-32-8	3028-33-9
	3028-34-0	3028-35-1	3028-36-2	3028-37-3	3028-38-4
	3028-39-5	3028-40-8	3028-41-9	3028-42-0	3028-43-1
	3028-44-2	3028-45-3	3028-46-4	3028-47-5	3028-48-6
	3028-49-7	3028-50-0	3028-51-1	3028-52-2	3028-53-3
	3028-54-4	3028-55-5	3028-56-6	3028-57-7	3028-58-8
	3028-59-9	3028-60-2	3028-63-5	3028-64-6	3028-65-7
	3028-66-8	3028-67-9	3028-68-0	3028-69-1	3028-70-4
	3028-71-5	3028-72-6	3028-73-7	3061-79-8	3065-35-8
	3065-36-9	3089-74-5	3089-80-3	3089-81-4	3089-82-5
	3374-09-2	3374-10-5	3441-66-5	3441-76-7	3441-77-8
	3441-78-9	3441-79-0	3442-16-8	3577-41-1	3577-42-2
	3978-36-7				

L111 ANSWER 4 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA62:3997g CAOLD

TITLE: intramol. cyclization of alkylpropargyldenemalonic acids-catalytic and directing effect of Ag ion

AUTHOR NAME: Belil, C.; Pascual, J.; Serratosa, F.

INDEX TERM: 921-46-0 921-86-8 922-87-2 922-90-7

924-95-8 936-09-4 946-67-8 1069-35-8

1137-22-0 1186-86-3 1196-35-6

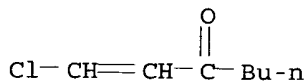
1213-20-3 1920-22-5 2052-89-3

IT 924-95-8 1137-22-0 1186-86-3

1920-22-5

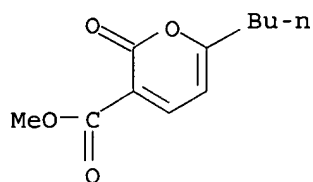
RN 924-95-8 CAOLD

CN 1-Hepten-3-one, 1-chloro- (7CI, 8CI, 9CI) (CA INDEX NAME)

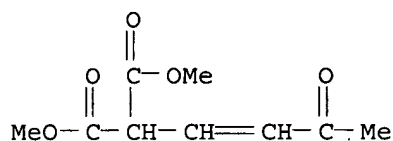


RN 1137-22-0 CAOLD

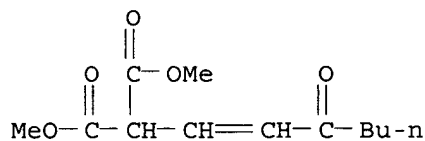
CN Malonic acid, (3-hydroxy-2-heptenylidene)-, δ -lactone, methyl ester (7CI, 8CI) (CA INDEX NAME)



RN 1186-86-3 CAOLD
 CN Malonic acid, (3-oxo-1-butenyl)-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)



RN 1920-22-5 CAOLD
 CN Malonic acid, (3-oxo-1-heptenyl)-, dimethyl ester (7CI, 8CI) (CA INDEX NAME)



IT 921-46-0 921-86-8 922-87-2
 922-90-7 924-95-8 936-09-4 946-67-8 1069-35-8
 1137-22-0 1186-86-3 1196-35-6 1213-20-3 1920-22-5
 2052-89-3

L111 ANSWER 5 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA62:2717b CAOLD

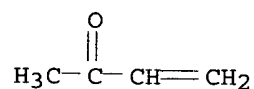
TITLE: course of the Michael aldol synthesis - (I)
 formation of cyclopentanediones, (II) of
 cyclohexenones

AUTHOR NAME: Goldsmith, David J.; Hartman, J. A.

INDEX TERM: 78-94-4 183-97-1 759-65-9
 765-70-8 769-45-9 769-46-0 771-74-4
 778-06-3 780-73-4 783-70-0
 786-14-1 889-67-8 26103-79-7
 91062-15-6 92723-62-1 94520-21-5
 96080-97-6 96380-22-2

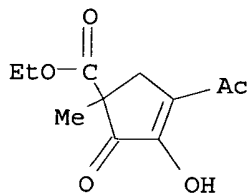
IT 78-94-4 780-73-4 783-70-0
 786-14-1 26103-79-7 92723-62-1
 96380-22-2

RN 78-94-4 CAOLD
 CN 3-Buten-2-one (8CI, 9CI) (CA INDEX NAME)



RN 780-73-4 CAOLD

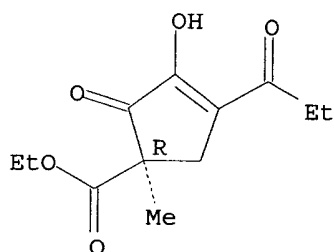
CN 3-Cyclopentene-1-carboxylic acid, 4-acetyl-3-hydroxy-1-methyl-2-oxo-, ethyl ester (7CI, 8CI) (CA INDEX NAME)



RN 783-70-0 CAOLD

CN 3-Cyclopentene-1-carboxylic acid, 3-hydroxy-1-methyl-2-oxo-4-propionyl-, ethyl ester, (R)- (8CI) (CA INDEX NAME)

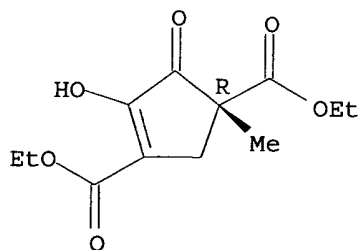
Absolute stereochemistry.



RN 786-14-1 CAOLD

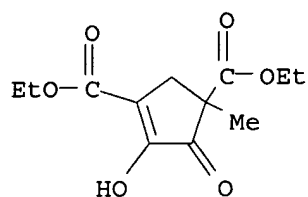
CN 3-Cyclopentene-1,3-dicarboxylic acid, 4-hydroxy-1-methyl-5-oxo-, diethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

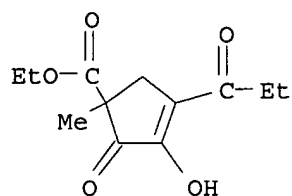


RN 26103-79-7 CAOLD

CN 3-Cyclopentene-1,3-dicarboxylic acid, 4-hydroxy-1-methyl-5-oxo-, diethyl ester (7CI, 9CI) (CA INDEX NAME)



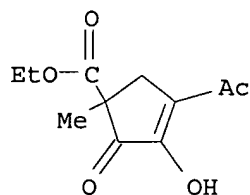
RN 92723-62-1 CAOLD
 CN 3-Cyclopentene-1-carboxylic acid, 3-hydroxy-1-methyl-2-oxo-4-propionyl-, ethyl ester (7CI) (CA INDEX NAME)



RN 96380-22-2 CAOLD
 CN 3-Cyclopentene-1-carboxylic acid, 4-acetyl-3-hydroxy-1-methyl-2-oxo-, ethyl ester, semicarbazone (7CI) (CA INDEX NAME)

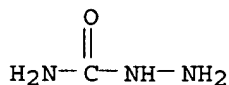
CM 1

CRN 780-73-4
 CMF C11 H14 O5



CM 2

CRN 57-56-7
 CMF C H5 N3 O



IT 78-94-4 183-97-1 759-65-9
 765-70-8 769-45-9 769-46-0
 771-74-4 778-06-3 780-73-4 783-70-0 786-14-1
 889-67-8 26103-79-7 91062-15-6 92723-62-1 94520-21-5
 96080-97-6 96380-22-2

L111 ANSWER 6 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA61:7827h CAOLD

TITLE: least-sqs. local-energy method for mol.-energy level calcn.

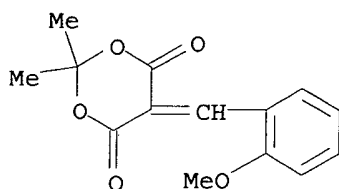
AUTHOR NAME: Frost, Arthur A.

INDEX TERM: 922-64-5 1214-54-6 2826-28-0 4335-90-4
5381-33-9 15795-54-7 **15795-56-9**
15795-57-0 15875-48-6 15875-49-7 17474-27-0
20444-83-1 20444-87-5 **22163-77-5**
23111-03-7 23340-25-2 23340-26-3 26187-43-9
68588-31-8 90536-56-4 91688-54-9 94546-37-9
95218-82-9

IT **15795-56-9 22163-77-5**

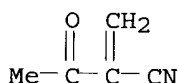
RN 15795-56-9 CAOLD

CN 1,3-Dioxane-4,6-dione, 5-[(2-methoxyphenyl)methylene]-2,2-dimethyl-
(9CI) (CA INDEX NAME)



RN 22163-77-5 CAOLD

CN Butanenitrile, 2-methylene-3-oxo- (9CI) (CA INDEX NAME)



IT **922-64-5 1214-54-6 2826-28-0 4335-90-4**
5381-33-9 15795-54-7 15795-56-9 15795-57-0 15875-48-6
15875-49-7 17474-27-0 20444-83-1 20444-87-5 22163-77-5
23111-03-7 23340-25-2 23340-26-3 26187-43-9 68588-31-8
90536-56-4 91688-54-9 94546-37-9 95218-82-9

L111 ANSWER 7 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA61:7047h CAOLD

TITLE: elimination - (VII) syntheses of DL-piperitone
(DL-p-menthen-3-one) and related compds. from
tert-butyl β -oxo esters

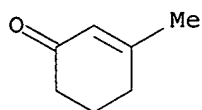
AUTHOR NAME: Lawesson, Sven O.; Larsen, E. H.; Jakobsen, H. J.;
Frisell, C.

INDEX TERM: **1193-18-6 93043-68-6**
94092-64-5 94428-39-4

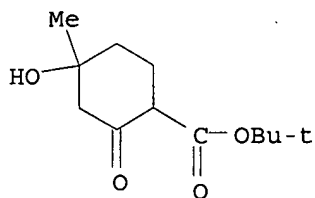
IT **1193-18-6 93043-68-6 94092-64-5**
94428-39-4

RN 1193-18-6 CAOLD

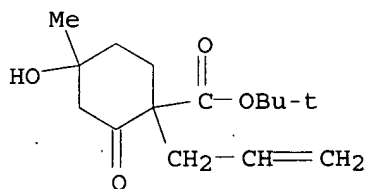
CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



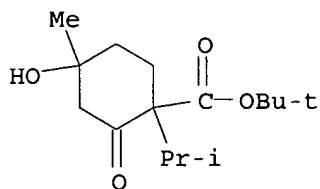
RN 93043-68-6 CAOLD
CN Cyclohexanecarboxylic acid, 4-hydroxy-4-methyl-2-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)



RN 94092-64-5 CAOLD
CN Cyclohexanecarboxylic acid, 1-allyl-4-hydroxy-4-methyl-2-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)



RN 94428-39-4 CAOLD
CN p-Menthane-4-carboxylic acid, 1-hydroxy-3-oxo-, tert-butyl ester (7CI) (CA INDEX NAME)



IT 1193-18-6 93043-68-6 94092-64-5
94428-39-4

L111 ANSWER 8 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA60:7926c CAOLD

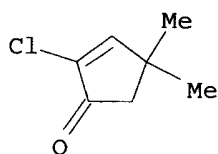
TITLE: halogen-substituted 1,3-cyclohexanediones - (I)
reaction of 2,2-dichlorodimedon with bases, (II)
chlorinated cycloalkanones from 2,2-dichlorodimedon

AUTHOR NAME: Schamp, N.; Verzele, M.

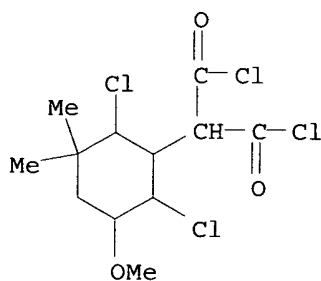
INDEX TERM: 932-23-0 7298-86-4 10545-47-8 17257-68-0
17530-72-2 17530-74-4 17530-75-5

17554-69-7 17554-71-1 17554-72-2
 17554-73-3 17554-76-6 17554-77-7 17554-78-8
 17554-86-8 17554-87-9 90153-71-2
 90560-70-6 93718-10-6

IT 17554-69-7 90560-70-6
 RN 17554-69-7 CAOLD
 CN 2-Cyclopenten-1-one, 2-chloro-4,4-dimethyl- (7CI, 8CI, 9CI) (CA INDEX NAME)

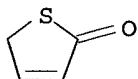


RN 90560-70-6 CAOLD
 CN Cyclohexanemalonyl chloride, 2,6-dichloro-3-methoxy-5,5-dimethyl- (7CI) (CA INDEX NAME)

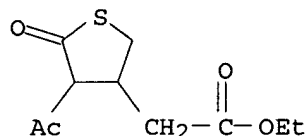


IT 932-23-0 7298-86-4 10545-47-8 17257-68-0
 17530-72-2 17530-74-4 17530-75-5 17554-69-7 17554-71-1
 17554-72-2 17554-73-3 17554-76-6 17554-77-7 17554-78-8
 17554-86-8 17554-87-9 90153-71-2 90560-70-6 93718-10-6

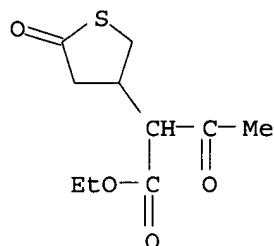
L111 ANSWER 9 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: CA59:12740c CAOLD
 TITLE: thiophene chemistry - (VIII) Michael addns. to
 2(5H)-thiophenone
 AUTHOR NAME: Jakobsen, Hans J.; Larsen, E. H.; Lawesson, S. O.
 INDEX TERM: 3354-32-3 94520-69-1
 98840-40-5
 IT 3354-32-3 94520-69-1 98840-40-5
 RN 3354-32-3 CAOLD
 CN 2(5H)-Thiophenone (8CI, 9CI) (CA INDEX NAME)



RN 94520-69-1 CAOLD
 CN Glutaric acid, 2-acetyl-3-(mercaptomethyl)-, 1-ethyl ester,
 γ-(thiolactone) (7CI) (CA INDEX NAME)



RN 98840-40-5 CAOLD
 CN 3-Thiopheneacetic acid, α -acetyltetrahydro-5-oxo-, ethyl ester (7CI) (CA INDEX NAME)



IT 3354-32-3 94520-69-1 98840-40-5

L111 ANSWER 10 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA59:6374h CAOLD

TITLE: total synthesis of the antibiotics thiolutin and holomycin

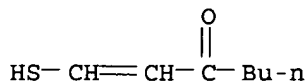
AUTHOR NAME: Schmidt, Ulrich; Geiger, F.

INDEX TERM: 87-11-6 488-04-0 17771-36-7 17771-37-8
 17771-38-9 17958-78-0 40647-81-2 40970-25-0
 40970-28-3 40970-29-4 61040-21-9 82031-42-3
 86247-90-7 89531-66-8 **89896-91-3**
 90345-39-4 90438-00-9 90612-05-8 90770-46-0
 91013-69-3 91558-95-1 91807-18-0 92369-67-0
 92576-32-4 92851-68-8 **93041-65-7**
 93139-36-7 93262-81-8 93427-67-9 93689-26-0
 94000-31-4 94488-37-6 94501-89-0 94584-10-8
 95591-82-5 95875-90-4 95937-27-2 96775-79-0
 96792-79-9 96951-63-2 97236-85-6 97525-12-7
 97525-48-9 98000-64-7 98529-76-1 100152-96-3
 106599-90-0

IT **89896-91-3** **93041-65-7**

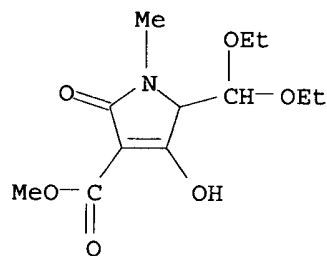
RN 89896-91-3 CAOLD

CN 1-Hepten-3-one, 1-mercapto- (7CI) (CA INDEX NAME)



RN 93041-65-7 CAOLD

CN 3-Pyrroline-3-carboxylic acid, 5-formyl-4-hydroxy-1-methyl-2-oxo-, methyl ester, diethyl acetal (7CI) (CA INDEX NAME)



IT 87-11-6 488-04-0 17771-36-7 17771-37-8
 17771-38-9 17958-78-0 40647-81-2 40970-25-0 40970-28-3
 40970-29-4 61040-21-9 82031-42-3 86247-90-7 89531-66-8
 89896-91-3 90345-39-4 90438-00-9 90612-05-8 90770-46-0
 91013-69-3 91558-95-1 91807-18-0 92369-67-0 92576-32-4
 92851-68-8 93041-65-7 93139-36-7 93262-81-8 93427-67-9
 93689-26-0 94000-31-4 94488-37-6 94501-89-0 94584-10-8
 95591-82-5 95875-90-4 95937-27-2 96775-79-0 96792-79-9
 96951-63-2 97236-85-6 97525-12-7 97525-48-9 98000-64-7
 98529-76-1 100152-96-3 106599-90-0

L111 ANSWER 11 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA59:585b CAOLD

TITLE: condensation reactions with isoxazoles-extension of the Ritter reaction

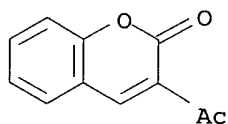
AUTHOR NAME: Eugster, Conrad H.; Leichner, L.; Jenny, E.

INDEX TERM: 3949-36-8 6317-31-3 17433-51-1
 18938-02-8 23340-25-2 33185-16-9 42222-06-0
 43135-05-3 57524-14-8 63879-04-9 72152-84-2
 73661-48-0 78450-21-2 78450-22-3 88590-04-9
 89379-78-2 89809-70-1 90347-95-8
 90565-41-6 90978-55-5 91137-31-4 91240-33-4
 91251-51-3 91251-95-5 91252-52-7 91253-23-5
 91253-30-4 91333-88-9 91718-35-3 92027-20-8
 92151-50-3 92188-50-6 92244-26-3 92646-74-7
 92652-35-2

IT 3949-36-8 89379-78-2

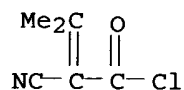
RN 3949-36-8 CAOLD

CN 2H-1-Benzopyran-2-one, 3-acetyl- (9CI) (CA INDEX NAME)



RN 89379-78-2 CAOLD

CN Crotonoyl chloride, 2-cyano-3-methyl- (6CI, 7CI) (CA INDEX NAME)



IT 3949-36-8 6317-31-3 17433-51-1 18938-02-8
 23340-25-2 33185-16-9 42222-06-0 43135-05-3 57524-14-8

63879-04-9 72152-84-2 73661-48-0 78450-21-2 78450-22-3
88590-04-9 89379-78-2 89809-70-1 90347-95-8 90565-41-6
90978-55-5 91137-31-4 91240-33-4 91251-51-3 91251-95-5
91252-52-7 91253-23-5 91253-30-4 91333-88-9 91718-35-3
92027-20-8 92151-50-3 92188-50-6 92244-26-3 92646-74-7
92652-35-2

L111 ANSWER 12 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA58:9420e CAOLD

TITLE: effects of chemicals on the mitotic cell in
plant-tropoids

AUTHOR NAME: Shimizu, Yoshitaka

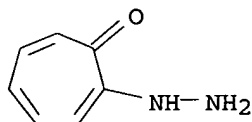
INDEX TERM: 363-67-7 641-28-1 698-18-0
1210-27-1 2132-33-4 2161-21-9 2161-40-2
2161-45-7 2229-97-2 2745-10-0 3331-45-1
3336-70-7 3336-74-1 3480-08-8 3525-04-0
3525-06-2 3525-13-1 3806-02-8
3839-48-3 4481-35-0 6264-93-3
6422-12-4 6504-36-5 7009-19-0 7021-46-7
15852-41-2 21473-91-6 21505-60-2 22442-46-2
23957-64-4 25946-69-4 27571-10-4 33739-56-9
33756-57-9 33902-86-2 36039-41-5
36044-38-9 50472-20-3 50472-24-7 51163-64-5
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89583-83-5 89975-62-2 89976-57-8
90005-81-5 90035-67-9 90326-38-8 90557-54-3
90560-17-1 90560-38-6 90766-32-8 90770-92-6
90887-13-1 90914-87-7 90922-80-8 91091-48-4
91805-09-3 91820-16-5 91955-17-8 91983-38-9
91997-34-1 91997-52-3 92026-81-8 92248-31-2
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92819-49-3 92847-26-2 92850-76-5
92959-86-9 93008-66-3 93011-82-6
93187-11-2 93353-13-0 93738-09-1 93817-25-5
94269-56-4 94296-56-7 94303-45-4 94378-21-9
94488-35-4 94673-71-9 94997-50-9 95140-61-7
95163-70-5 95767-12-7 95767-13-8 97980-17-1
98494-99-6 100196-33-6 100232-84-6 102924-42-5
104879-21-2

IT 698-18-0 3839-48-3 6264-93-3

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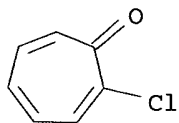
RN 698-18-0 CAOLD

CN 2,4,6-Cycloheptatrien-1-one, 2-hydrazino- (7CI, 8CI, 9CI) (CA
INDEX NAME)

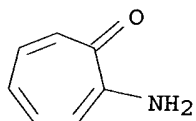


RN 3839-48-3 CAOLD

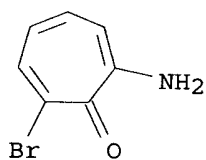
CN 2,4,6-Cycloheptatrien-1-one, 2-chloro- (6CI, 7CI, 8CI, 9CI) (CA
INDEX NAME)



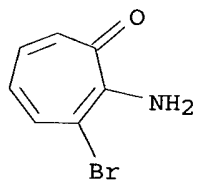
RN 6264-93-3 CAOLD
 CN 2,4,6-Cycloheptatrien-1-one, 2-amino- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



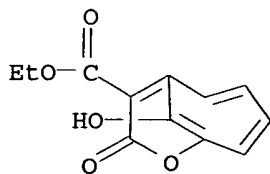
RN 36039-41-5 CAOLD
 CN 2,4,6-Cycloheptatrien-1-one, 2-amino-7-bromo- (7CI, 9CI) (CA INDEX NAME)



RN 89975-62-2 CAOLD
 CN 2,4,6-Cycloheptatrien-1-one, 2-amino-3-bromo- (6CI, 7CI) (CA INDEX NAME)



RN 92959-86-9 CAOLD
 CN 2,4,6-Cycloheptatriene-Δ1,α-malonic acid, 2,3-dihydroxy-, δ-lactone, ethyl ester (7CI) (CA INDEX NAME)



IT 363-67-7 641-28-1 698-18-0
1210-27-1 2132-33-4 2161-21-9
2161-40-2 2161-45-7 2229-97-2 2745-10-0 3331-45-1
3336-70-7 3336-74-1 3480-08-8 3525-04-0 3525-06-2
3525-13-1 3806-02-8 3839-48-3 4481-35-0 6264-93-3
6422-12-4 6504-36-5 7009-19-0 7021-46-7 15852-41-2
21473-91-6 21505-60-2 22442-46-2 23957-64-4 25946-69-4
27571-10-4 33739-56-9 33756-57-9 33902-86-2 36039-41-5
36044-38-9 50472-20-3 50472-24-7 51163-64-5 67931-57-1
86371-89-3 88614-27-1 88614-51-1 89583-83-5 89975-62-2
89976-57-8 90005-81-5 90035-67-9 90326-38-8 90557-54-3
90560-17-1 90560-38-6 90766-32-8 90770-92-6 90887-13-1
90914-87-7 90922-80-8 91091-48-4 91805-09-3 91820-16-5
91955-17-8 91983-38-9 91997-34-1 91997-52-3 92026-81-8
92248-31-2 92254-30-3 92288-77-2 92381-56-1 92765-09-8
92819-49-3 92847-26-2 92850-76-5 92959-86-9 93008-66-3
93011-82-6 93187-11-2 93353-13-0 93738-09-1 93817-25-5
94269-56-4 94296-56-7 94303-45-4 94378-21-9 94488-35-4
94673-71-9 94997-50-9 95140-61-7 95163-70-5 95767-12-7
95767-13-8 97980-17-1 98494-99-6 100196-33-6 100232-84-6
102924-42-5 104879-21-2

L111 ANSWER 13 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA58:9067c CAOLD

TITLE: carboxylic acid derivs. - (V) ketene derivs. (I)
substituted dithiocarboxylic acids and ketene
mercaptals, (II) reactions of substituted ketene
mercaptals, (III) pyrazoles and isoxazoles from
ketene mercaptals

AUTHOR NAME: Gompper, Rudolf; Toepfl, W.

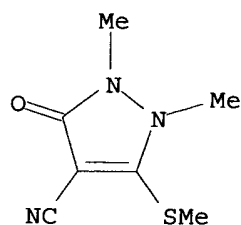
INDEX TERM: 2080-43-5 2276-43-9 2939-72-2 3490-92-4
4933-40-8 5147-80-8 5624-24-8 10354-92-4
10355-19-8 17823-64-2 17823-65-3 17823-69-7
18071-20-0 19607-08-0 23858-31-3 25241-08-1
25241-12-7 29866-36-2 29866-38-4 37614-61-2
37758-35-3 51531-96-5 51532-03-7 52046-75-0
52793-49-4 59334-11-1 60312-08-5 63114-05-6
68313-63-3 72760-85-1 81385-18-4 85106-72-5
88550-49-6 88614-56-6 89489-55-4
89853-59-8 90434-81-4 90771-90-7
90842-90-3 90916-95-3 91058-84-3
91134-34-8 91134-83-7 91807-27-1
91912-29-7 91974-70-8 92289-68-4 92548-31-7
92723-91-6 92801-12-2 92964-02-8
93013-94-6 94031-91-1 94066-35-0 94267-21-7
94933-83-2 94982-52-2 95533-91-8
95697-30-6 96329-56-5 97103-00-9 97299-68-8
97441-93-5 97595-95-4 97595-96-5 97725-92-3
97980-57-9 99996-85-7 100168-89-6

IT 89853-59-8 91134-34-8 91134-83-7

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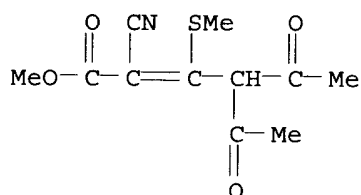
RN 89853-59-8 CAOLD

CN 3-Pyrazoline-4-carbonitrile, 1,2-dimethyl-3-(methylthio)-5-oxo-
(7CI) (CA INDEX NAME)



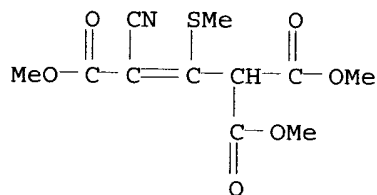
RN 91134-34-8 CAOLD

CN 2-Hexenoic acid, 4-acetyl-2-cyano-3-(methylthio)-5-oxo-, methyl ester (7CI) (CA INDEX NAME)



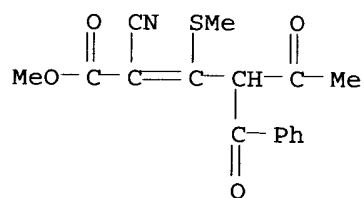
RN 91134-83-7 CAOLD

CN 2-Propene-1,1,3-tricarboxylic acid, 3-cyano-2-(methylthio)-, trimethyl ester (7CI) (CA INDEX NAME)



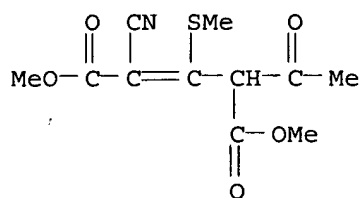
RN 92964-02-8 CAOLD

CN 2-Hexenoic acid, 4-benzoyl-2-cyano-3-(methylthio)-5-oxo-, methyl ester (7CI) (CA INDEX NAME)



RN 94982-52-2 CAOLD

CN Glutaconic acid, 4-acetyl-2-cyano-3-(methylthio)-, dimethyl ester (7CI) (CA INDEX NAME)



IT	2080-43-5	2276-43-9	2939-72-2	
	3490-92-4	4933-40-8	5147-80-8	5624-24-8
	10354-92-4	10355-19-8	17823-64-2	17823-65-3 17823-69-7
	18071-20-0	19607-08-0	23858-31-3	25241-08-1 25241-12-7
	29866-36-2	29866-38-4	37614-61-2	37758-35-3 51531-96-5
	51532-03-7	52046-75-0	52793-49-4	59334-11-1 60312-08-5
	63114-05-6	68313-63-3	72760-85-1	81385-18-4 85106-72-5
	88550-49-6	88614-56-6	89489-55-4	89853-59-8 90434-81-4
	90771-90-7	90842-90-3	90916-95-3	91058-84-3 91134-34-8
	91134-83-7	91807-27-1	91912-29-7	91974-70-8 92289-68-4
	92548-31-7	92723-91-6	92801-12-2	92964-02-8 93013-94-6
	94031-91-1	94066-35-0	94267-21-7	94933-83-2 94982-52-2
	95533-91-8	95697-30-6	96329-56-5	97103-00-9 97299-68-8
	97441-93-5	97595-95-4	97595-96-5	97725-92-3 97980-57-9
	99996-85-7	100168-89-6		

L111 ANSWER 14 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA58:5529a CAOLD

TITLE: elimination - (V) synthesis of 1-methyl-1-cyclohexen-3-one and related compds.

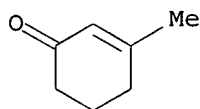
AUTHOR NAME: Naslund, Gunnell; Senning, A.; Lawesson, S. O.

INDEX TERM: 1193-18-6 5715-25-3 94329-15-4
94801-98-6 95169-78-1 95557-23-6
96171-90-3 96268-73-4

IT 1193-18-6 94801-98-6

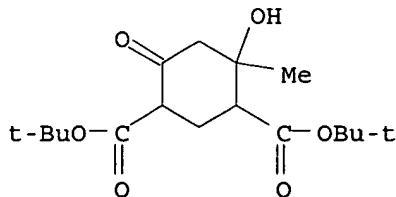
RN 1193-18-6 CAOLD

CN 2-Cyclohexen-1-one, 3-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 94801-98-6 CAOLD

CN 1,3-Cyclohexanedicarboxylic acid, 4-hydroxy-4-methyl-6-oxo-, di-tert-butyl ester (7CI) (CA INDEX NAME)



IT 1193-18-6 5715-25-3 94329-15-4 94801-98-6

95169-78-1 95557-23-6 96171-90-3 96268-73-4

L111 ANSWER 15 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA56:9998g CAOLD

TITLE: synthesis of terpenes - (VII) 9-methyl-6-oxo-
Δ⁴(10)-1-octahydro-naphthyleneacetic acid

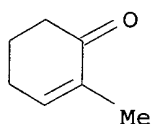
AUTHOR NAME: Davis, Brian Reeve; Gupta, S. R.; Halsall, T. G.

INDEX TERM: 1121-18-2 6272-53-3
37457-15-1 57026-73-0 65093-74-5 90975-34-1
91966-06-2 92730-34-2 93726-57-9 94092-45-2
95556-08-4 97261-87-5

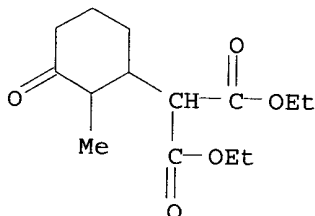
IT 1121-18-2 6272-53-3

RN 1121-18-2 CAOLD

CN 2-Cyclohexen-1-one, 2-methyl- (7CI, 8CI, 9CI) (CA INDEX NAME)



RN 6272-53-3 CAOLD

CN Propanedioic acid, (2-methyl-3-oxocyclohexyl)-, diethyl ester
(9CI) (CA INDEX NAME)IT 1121-18-2 6272-53-3 37457-15-1 57026-73-0
65093-74-5 90975-34-1 91966-06-2 92730-34-2 93726-57-9
94092-45-2 95556-08-4 97261-87-5

L111 ANSWER 16 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA55:19918d CAOLD

TITLE: aromaticity by nuclear resonance spectroscopy - (I)
2-pyridones and related systems

AUTHOR NAME: Elvidge, J. A.; Jackman, L. M.

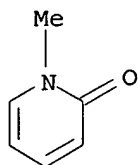
INDEX TERM: 689-89-4 694-85-9 1003-56-1
1149-24-2 1150-55-6 6456-92-4
6456-93-5 15031-43-3 15031-89-7
15827-70-0 22739-24-8 31349-63-0 39594-85-9
100610-52-4 109103-38-0 111063-62-8
132778-74-6

IT 694-85-9 6456-92-4 6456-93-5

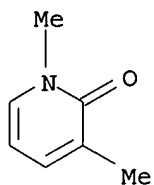
15031-43-3 100610-52-4

RN 694-85-9 CAOLD

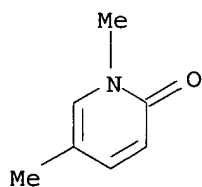
CN 2(1H)-Pyridinone, 1-methyl- (9CI) (CA INDEX NAME)



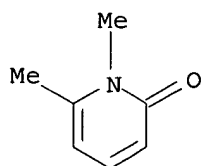
RN 6456-92-4 CAOLD
CN 2(1H)-Pyridinone, 1,3-dimethyl- (9CI) (CA INDEX NAME)



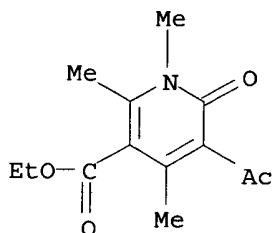
RN 6456-93-5 CAOLD
CN 2(1H)-Pyridinone, 1,5-dimethyl- (9CI) (CA INDEX NAME)



RN 15031-43-3 CAOLD
CN 2(1H)-Pyridinone, 1,6-dimethyl- (9CI) (CA INDEX NAME)



RN 100610-52-4 CAOLD
CN Nicotinic acid, 5-acetyl-1,6-dihydro-1,2,4-trimethyl-6-oxo-, ethyl ester (6CI) (CA INDEX NAME)



IT 689-89-4 694-85-9 1003-56-1
 1149-24-2 1150-55-6 6456-92-4 6456-93-5
 15031-43-3 15031-89-7 15827-70-0 22739-24-8 31349-63-0
 39594-85-9 100610-52-4 109103-38-0 111063-62-8 132778-74-6

L111 ANSWER 17 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA53:332a CAOLD

TITLE: active components of *Digenea simplex* and related
 compds. - (LIV) synthesis of 2-carboxy-3-
 pyrrolidineacetic acid (2-i), (LV) (2-ii), (LVI) of
 L- α -dihydrokainic acid (2-i), (LVII) (2-ii),
 (LVIII) of L- α -allokainic acid (3)

AUTHOR NAME: Sugawa, Toshio

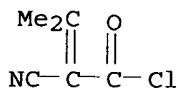
INDEX TERM: 759-21-7 3731-16-6 10444-38-9 14869-34-2
 17216-62-5 49785-86-6 58474-93-4
89379-78-2 89775-98-4 90979-03-6
 93273-12-2 **93432-60-1** 96229-51-5
 97497-60-4 98133-48-3 98140-80-8 98491-69-1
 98547-29-6 99075-65-7 99076-43-4 99076-47-8
 99176-40-6 99189-77-2 100132-48-7 100453-82-5
 101020-91-1 101086-73-1 **101086-74-2**
 101109-05-1 101568-82-5 101589-43-9 101777-53-1
 101867-55-4 102015-01-0 102074-21-5 102708-95-2
 102878-66-0 104743-70-6 104912-63-2 106163-77-3
 106275-34-7 **107777-89-9** 107923-09-1
 108085-38-7 **108479-31-8** 109162-12-1
 109731-65-9 111007-80-8 112441-11-9 117343-07-4
 119417-53-7 131241-49-1

IT 89379-78-2 93432-60-1 101086-74-2

107777-89-9 108479-31-8

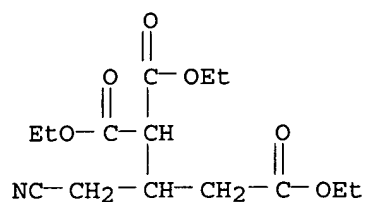
RN 89379-78-2 CAOLD

CN Crotonoyl chloride, 2-cyano-3-methyl- (6CI, 7CI) (CA INDEX NAME)

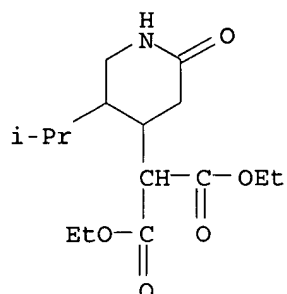


RN 93432-60-1 CAOLD

CN 1,1,3-Propanetricarboxylic acid, 2-(cyanomethyl)-, triethyl ester
 (6CI, 7CI) (CA INDEX NAME)

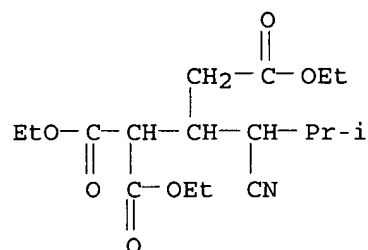


RN 101086-74-2 CAOLD

CN 4-Piperidinemalonic acid, 5-isopropyl-2-oxo-, diethyl ester (6CI)
(CA INDEX NAME)

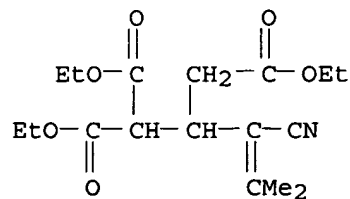
RN 107777-89-9 CAOLD

CN 1,1,3-Propanetricarboxylic acid, 2-(1-cyano-2-methylpropyl)-, triethyl ester (6CI) (CA INDEX NAME)



RN 108479-31-8 CAOLD

CN 1,1,3-Propanetricarboxylic acid, 2-(1-cyano-2-methylpropenyl)-, triethyl ester (6CI) (CA INDEX NAME)

IT 759-21-7 3731-16-6 10444-38-9
14869-34-2 17216-62-5 49785-86-6 58474-93-4

89379-78-2 89775-98-4 90979-03-6 93273-12-2 93432-60-1
 96229-51-5 97497-60-4 98133-48-3 98140-80-8 98491-69-1
 98547-29-6 99075-65-7 99076-43-4 99076-47-8 99176-40-6
 99189-77-2 100132-48-7 100453-82-5 101020-91-1 101086-73-1
 101086-74-2 101109-05-1 101568-82-5 101589-43-9 101777-53-1
 101867-55-4 102015-01-0 102074-21-5 102708-95-2 102878-66-0
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 107923-09-1 108085-38-7 108479-31-8 109162-12-1 109731-65-9
 111007-80-8 112441-11-9 117343-07-4 119417-53-7 131241-49-1

L111 ANSWER 18 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA52:2848h CAOLD

TITLE: organic reactions with polyphosphoric acid - (V)
 intramol. acylation with lactones-cyclopentenones
 from α -lactones

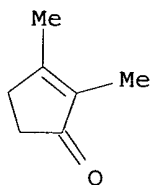
AUTHOR NAME: Dev, Sukh; Rai, C.

INDEX TERM: 1121-05-7 1572-39-0 1572-40-3
 2275-26-5 3296-45-5 4430-31-3 6053-92-5
 6818-07-1 10413-18-0 22117-99-3 22118-00-9
 57026-64-9 84196-94-1 89244-93-9
 93865-05-5 110061-30-8 116154-62-2

IT 1121-05-7 57026-64-9 93865-05-5

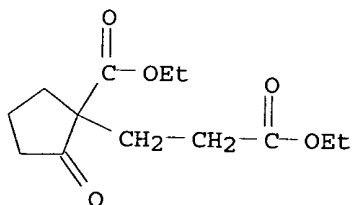
RN 1121-05-7 CAOLD

CN 2-Cyclopenten-1-one, 2,3-dimethyl- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



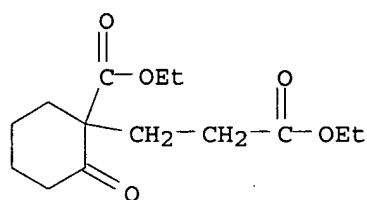
RN 57026-64-9 CAOLD

CN Cyclopentanepropanoic acid, 1-(ethoxycarbonyl)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



RN 93865-05-5 CAOLD

CN Cyclohexanepropanoic acid, 1-(ethoxycarbonyl)-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



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 10413-18-0 22117-99-3 22118-00-9 57026-64-9 84196-94-1
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L111 ANSWER 19 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA51:15699h CAOLD

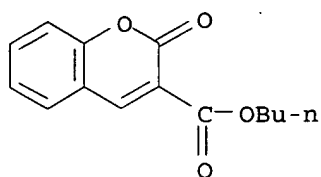
TITLE: synthetic compds. active against Salmonella
 dysentery group bacilli

AUTHOR NAME: Akiya, Shichiro

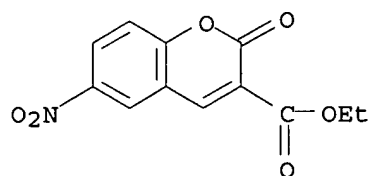
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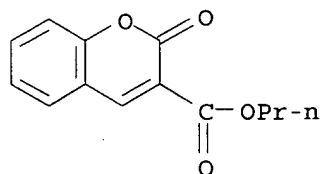
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101090-86-2 116890-40-5 117756-51-1
RN 7460-87-9 CAOLD
CN 2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, butyl ester (6CI, 9CI)
(CA INDEX NAME)



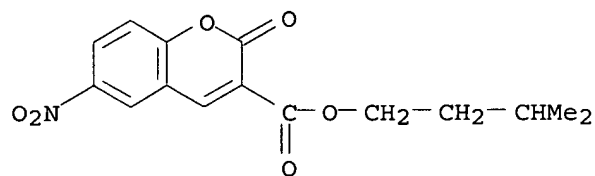
RN 13373-28-9 CAOLD

CN 2H-1-Benzopyran-3-carboxylic acid, 6-nitro-2-oxo-, ethyl ester
(6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

RN 39497-12-6 CAOLD

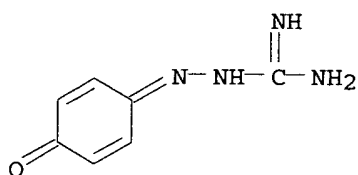
CN 2H-1-Benzopyran-3-carboxylic acid, 2-oxo-, propyl ester (6CI, 9CI)
(CA INDEX NAME)

RN 101090-86-2 CAOLD

CN 2H-1-Benzopyran-3-carboxylic acid, 6-nitro-2-oxo-, isopentyl ester
(6CI) (CA INDEX NAME)

RN 116890-40-5 CAOLD

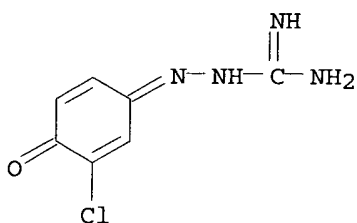
CN Guanidine, [(dichloro-4-oxo-2,5-cyclohexadien-1-ylidene)amino]-
(6CI) (CA INDEX NAME)



2 (D1- C1)

RN 117756-51-1 CAOLD

CN Guanidine, [(3-chloro-4-oxo-2,5-cyclohexadien-1-ylidene)amino]-(6CI) (CA INDEX NAME)



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L111 ANSWER 20 OF 21 CAOLD COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: CA51:12890c CAOLD

TITLE: reaction of β -chlorovinyl ketones with
 β -dicarbonyl compds. - (III) ketovinylation of
malonic ester-new synthesis of α -pyrones

AUTHOR NAME: Kochetkov, N. K.; Kudryashov, L. I.

INDEX TERM: 105-32-8 105-53-3 3306-07-8

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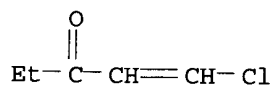
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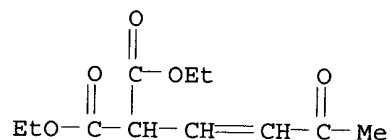
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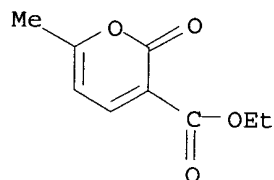
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CN Propanedioic acid, (3-oxo-1-butenyl)-, diethyl ester (9CI) (CA INDEX NAME)



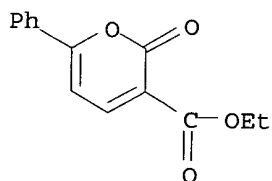
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CN 2H-Pyran-3-carboxylic acid, 6-methyl-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)



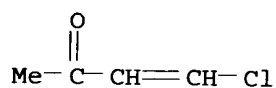
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CN 2H-Pyran-3-carboxylic acid, 2-oxo-6-phenyl-, ethyl ester (8CI, 9CI) (CA INDEX NAME)



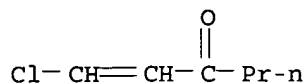
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CN 3-Buten-2-one, 4-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



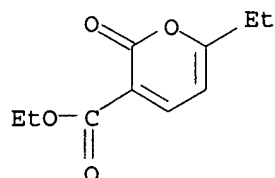
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CN 1-Hexen-3-one, 1-chloro- (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



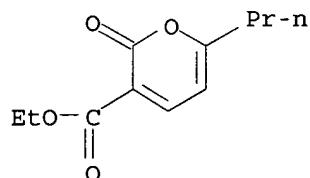
RN 99186-81-9 CAOLD

CN Malonic acid, (3-hydroxy-2-pentenylidene)-, δ -lactone, ethyl ester (6CI) (CA INDEX NAME)



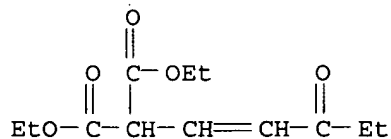
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CN Malonic acid, (3-hydroxy-2-hexenylidene)-, δ -lactone, ethyl ester (6CI) (CA INDEX NAME)



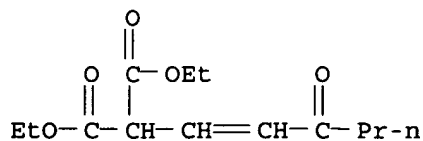
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CN Malonic acid, (3-oxo-1-pentenyl)-, diethyl ester (6CI) (CA INDEX NAME)



RN 100533-49-1 CAOLD

CN Malonic acid, (3-oxo-1-hexenyl)-, diethyl ester (6CI) (CA INDEX NAME)

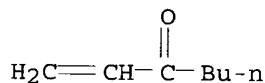


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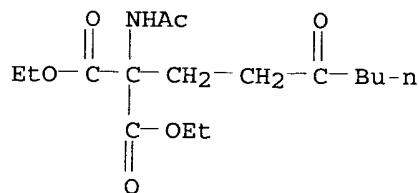
L111 ANSWER 21 OF 21 CAOLD COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: CA51:4439a CAOLD
 TITLE: 5-[2-(and 3)oxoalkyl]-2-thiohydantoins
 AUTHOR NAME: Archer, Sydney
 PATENT ASSIGNEE: Sterling Drug Inc.
 DOCUMENT TYPE: Patent

PATENT NO.	KIND	DATE
PI US 2763662		1956
INDEX TERM:	2918-13-0	4312-99-6 20261-68-1
	32831-00-8	39056-64-9 41055-92-9 41055-93-0
	41055-94-1	62005-96-3 63988-10-3 99419-66-6
	99459-61-7	100050-45-1 100247-74-3 100526-03-2
	100539-68-2	101252-26-0 101253-32-1
	101426-52-2	102154-84-7 102589-34-4
	102881-13-0	102882-11-1 103038-32-0 103040-05-7
	103152-42-7	103152-43-8 103155-35-7 103272-59-9
	103275-04-3	103393-59-5 103394-34-9 103395-08-0
	103396-17-4	104116-05-4 104116-51-0 107306-09-2
	109439-06-7	116080-78-5

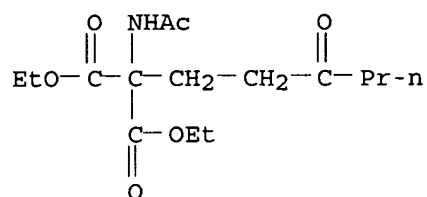
IT 2918-13-0 101426-52-2 109439-06-7
 RN 2918-13-0 CAOLD
 CN 1-Hepten-3-one (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)



RN 101426-52-2 CAOLD
 CN Malonic acid, acetamido(3-oxoheptyl)-, diethyl ester (6CI) (CA INDEX NAME)



RN 109439-06-7 CAOLD
 CN Malonic acid, acetamido(3-oxohexyl)-, diethyl ester (6CI) (CA INDEX NAME)



IT 2918-13-0 4312-99-6 20261-68-1
32831-00-8 39056-64-9 41055-92-9 41055-93-0 41055-94-1
62005-96-3 63988-10-3 99419-66-6 99459-61-7 100050-45-1
100247-74-3 100526-03-2 100539-68-2 101252-26-0 101253-32-1
101426-52-2 102154-84-7 102589-34-4 102881-13-0 102882-11-1
103038-32-0 103040-05-7 103152-42-7 103152-43-8 103155-35-7
103272-59-9 103275-04-3 103393-59-5 103394-34-9 103395-08-0
103396-17-4 104116-05-4 104116-51-0 107306-09-2 109439-06-7
116080-78-5

=> d que stat 199

L97 QUE ABB=ON PLU=ON (KANTO(W)KAGAKU?)/PA,CS,CO,SO
 L98 QUE ABB=ON PLU=ON WATANABE M?/AU OR MURATA K?/AU OR
 IKARIYA T?/AU
 L99 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L97 AND L98

=> d que stat 1104

L97 QUE ABB=ON PLU=ON (KANTO(W)KAGAKU?)/PA,CS,CO,SO
 L98 QUE ABB=ON PLU=ON WATANABE M?/AU OR MURATA K?/AU OR
 IKARIYA T?/AU
 L104 18 SEA L97 AND L98

=> d que stat 1105

L97 QUE ABB=ON PLU=ON (KANTO(W)KAGAKU?)/PA,CS,CO,SO
 L98 QUE ABB=ON PLU=ON WATANABE M?/AU OR MURATA K?/AU OR
 IKARIYA T?/AU
 L99 12 SEA FILE=HCAPLUS ABB=ON PLU=ON L97 AND L98
 L104 18 SEA L97 AND L98
 L105 18 DUP REM L99 L104 (12 DUPLICATES REMOVED)

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YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX' - CONTINUE? (Y)/N:y

L105 ANSWER 1 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 1
 ACCESSION NUMBER: 2005:207662 HCAPLUS
 DOCUMENT NUMBER: 142:297886
 TITLE: Process for preparing optically active nitro
 compounds and cyano compounds
 INVENTOR(S): **Watanabe, Masahito; Murata,**
Kunihiko; Ikariya, Takao
 PATENT ASSIGNEE(S): **Kanto Kagaku** Kabushiki
 Kaisha, Japan
 SOURCE: Eur. Pat. Appl., 35 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1512678	A1	20050309	EP 2004-20962	2004 0903
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
JP 2005187446	A2	20050714	JP 2004-76663	2004 0317
US 2005101787	A1	20050512	US 2004-934338	2004 0903

CN 1626501 A 20050615 CN 2004-10068730

2004
0906

PRIORITY APPLN. INFO.:

JP 2003-314096

A

2003
0905

JP 2003-407981

A

2003
1205

JP 2004-76663

A

2004
0317

OTHER SOURCE(S): CASREACT 142:297886; MARPAT 142:297886

ED Entered STN: 09 Mar 2005

AB Optically active nitro and cyano compds. (I) [wherein R1 = each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, hetero-mono- or polycyclic group, H, halogen, CO2H or its ester or amido, HO, alkoxy, NH2; R2, R3 = H, each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, or hetero-mono- or polycyclic group; X = NO2, cyano; or two of R1-R3 can form a ring binding each other; R4 = H, halogen, amido, amino, alkoxy, NO2, cyano, each (un)substituted aromatic mono- or polycyclic hydrocarbon, (un)saturated aliphatic or alicyclic hydrocarbon, or hetero-mono- or polycyclic group; R5, R6 = H, each (un)substituted aromatic mono- or polycyclic hydrocarbon, or (un)saturated aliphatic or alicyclic hydrocarbon group, straight or branched C1-20 alkoxy; or two of R4-R6 can form a ring binding each other; Y, Z = a single bond, O, S, N, P; m, n = 1, 2; in the case that Y and Z are a single bond, O or S atom, m and n are 1, and in the case that Y and Z are N or P atom, m and n are 2] are prepared in high efficiency and high stereoselectivity by simple and practical asym. Michael reaction of nitroethene or acrylonitrile derivs. (II) with dialkyl malonates or acylacetates (III) in the presence of a chiral metal complex, which is obtained by reaction of an optically active nitrogen-containing compound and a periodic table group VIII metal complex. Thus, [(S,S)-N-(2,4,6-triisopropylbenzenesulfonyl)-1,2-diphenylethylenediamine](hexamethylbenzene)ruthenium (14.8 mg, 0.02 mmol, S/C = 50), trans-p-nitrostyrene (149 mg, 1.0 mmol), di-Me malonate (114 µL, 1.0 mmol) and toluene (1 mL) were added into a Schlenk tube (20 mL) under an argon atmosphere, and stirred at 30° for 24 h to give, after purification by flash column chromatog. (hexane/acetone = 80/20, SiO2), 94% Me (R)-2-methoxycarbonyl-4-nitro-3-phenylbutanoate (87% ee).

IC ICM C07C255-22

ICS C07C205-53

CC 25-20 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 27, 29

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L105 ANSWER 2 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 2

ACCESSION NUMBER: 2004:584477 HCAPLUS

DOCUMENT NUMBER: 141:140101

TITLE: Process and catalysts for producing optically

INVENTOR(S): active cycloalkylmalonates
Watanabe, Masahito; Murata,
Kunihiko; Ikariya, Takao
PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki
Kaisha, Japan
SOURCE: Eur. Pat. Appl., 29 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	
EP 1439159	A1	20040721	EP 2004-296	2004 0109
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
JP 2004269481	A2	20040930	JP 2003-71368	2003 0317
US 2004176616	A1	20040909	US 2003-749806	2003 1231
PRIORITY APPLN. INFO.:			JP 2003-9786	A 2003 0117
			JP 2003-71368	A 2003 0317

OTHER SOURCE(S): MARPAT 141:140101

ED Entered STN: 22 Jul 2004

AB Optically active malonate derivs. R1COCR2R3CR4(COXR5)COYR6 [R1 = (un)substituted aromatic, aliphatic, alicyclic, heterocyclic, H, alkoxy, amino; R2-R4 = H, (un)substituted aryl, aliphatic, alicyclic, heterocyclic; R1R2, R1R3, R2R3, R4R5, R5R6, R4R6 = atoms required to form a ring; R5, R6 = H, (un)substituted aryl, aliphatic, alicyclic, alkoxy; X, Y = bond; XR5, YR6 = (un)substituted OH, NH2] were prepared by treating R1COCH:CR2R3 with R4CH(COXR5)COYR6 in presence of an asym. metal catalyst, preferably a Ru catalyst I [R7-R10 = (un)substituted Ph]. Thus, [RuCl2(C6Me6)]2 was treated with (S,S)-TsDPEN to give Ru[(S,S)-TsDPEN](C6Me6) which was used in the Michael reaction of 2-cyclohexenone with CH2(CO2Me)2 to give (R)-3-[bis(methoxycarbonyl)methyl]cyclohexanone in 96% ee.

IC ICM C07C045-72

CC 24-5 (Alicyclic Compounds)

L105 ANSWER 3 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 3

ACCESSION NUMBER: 2003:356091 HCAPLUS

DOCUMENT NUMBER: 138:353733

TITLE: Process for producing optically active amino alcohols

INVENTOR(S): Watanabe, Masahito; Murata,
Kunihiko; Ikariya, Takao

PATENT ASSIGNEE(S): Kanto Kagaku Kabushiki

SOURCE: Kaisha, Japan
Eur. Pat. Appl., 23 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1308435	A2	20030507	EP 2002-24517	2002 1030
EP 1308435	A3	20030604		
EP 1308435	B1	20051228		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, SK				
JP 2003201269	A2	20030718	JP 2002-251994	2002 0829
JP 3504254	B2	20040308		
CA 2409906	AA	20030430	CA 2002-2409906	2002 1028
JP 2003201270	A2	20030718	JP 2002-316217	2002 1030
US 2003171592	A1	20030911	US 2002-285164	2002 1031
US 6686505	B2	20040203		
PRIORITY APPLN. INFO.:			JP 2001-335322	A 2001 1031
			JP 2002-251994	A 2002 0829

OTHER SOURCE(S): MARPAT 138:353733

ED Entered STN: 09 May 2003

AB A process for producing an optically active amino alc. is provided that includes a step in which a nitro ketone or a cyano ketone is reacted with a hydrogen-donating organic or inorg. compound in the presence of a transition metal compound catalyst having an optically active nitrogen-containing compound as an asym. ligand to give an optically active nitro alc. or an optically active cyano alc., and a step in which the above optically active alc. is further reduced to efficiently produce an optically active amino alc. Thus, PhCOCH₂CN was reduced with HCO₂H in presence of Et₃N and chloro[(S,S)-N-(p-toluenesulfonyl)-1,2-diphenylethylenediamine](p-cymene)ruthenium to give (S)-HOCHPhCH₂CN in 98% ee. This compound was reduced with BH₃.Me₂S to give (S)-HOCHPhCH₂CH₂NH₂ with 98% ee. The alcs. are intermediates for pharmaceuticals, such as fluoxetine, tomoxetine, nioxetine and norfluoxetine.

IC ICM C07C201-12

ICS C07C253-30; C07C213-02

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

Section cross-reference(s): 27

L105 ANSWER 4 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 4
ACCESSION NUMBER: 1999:683209 HCAPLUS
DOCUMENT NUMBER: 131:310940
TITLE: Preparation method of bridged metallocene compounds
INVENTOR(S): Hori, Junichi; **Murata, Kunihiro**;
Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 11292891	A2	19991026	JP 1998-107170	1998 0403
PRIORITY APPLN. INFO.: JP 1998-107170				1998 0403

OTHER SOURCE(S): MARPAT 131:310940
ED Entered STN: 27 Oct 1999
AB Title compds., useful as catalysts for olefin polymerization or organic synthesis, are prepared by reaction of Group 4 transition metal compds. I and (M2)+(L1)-C(L2)-(M2)+ and are represented by the general formula II, where M1 = Group 4 transition metal; A = Group 15 or 16 heteroatom; B = Group 14 typical element; R1, R2 = (heteroatom-containing) C1-30 hydrocarbyl or H; X = halogen or O- or S-containing C1-10 group; p, q = 0, 1, or 2; p + q = 1 or 2; r = 1 or 2; s = 2 or 3; L1, L2 = (substituted) cyclopentadienyl, (substituted) indenyl, (substituted) azulenyl, or (substituted) fluorenyl; C = C1-20 hydrocarbyl, (C1-20 hydrocarbyl-containing) silylene, oligosilylene, or germirene; M2 = Group 1 or 2 typical metal; and t = s-2, etc. Halogenated metallocene compds. III (Y = halogen) are stereoselectively prepared from II. Thus, (N-methylanilide)zirconium trichloride bistetrahydrofuran was prepared from N-methylaniline, ZrCl4, and THF, and reacted with 1,2-bis(3-indenyl)ethane dilithium salt to give ethylenebis(1-indenyl)zirconium (N-methylanilide) chloride.
IC ICM C07F017-00
CC 35-3 (Chemistry of Synthetic High Polymers)
Section cross-reference(s): 29, 67

L105 ANSWER 5 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 5
ACCESSION NUMBER: 1999:680136 HCAPLUS
DOCUMENT NUMBER: 131:310939
TITLE: Organic transition metal chemical compound
INVENTOR(S): Hori, Junichi; **Murata, Kunihiro**;
Yoshida, Masahiro
PATENT ASSIGNEE(S): **Kanto Kagaku** K. K., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 37 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent

LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11292890	A2	19991026	JP 1998-107169	1998 0403

PRIORITY APPLN. INFO.: JP 1998-107169
 1998
 0403

OTHER SOURCE(S): MARPAT 131:310939

ED Entered STN: 26 Oct 1999

AB The title compds. comprise I (M = group 4 metal; A = group 15 heteroatom; B = Si, Ge, Sn, Pb; R1 = H, C1-20 hydrocarbyl which may contain heteroatoms; R2 = H, C1-20 hydrocarbyl; X = halogen; p, q = 0-2, p + q = 2; r = 1, 2; s = 2, 3, etc.).
 (N-Methylanilide)zirconium trichloride was prepared from N-methylaniline and ZrCl₄, then reacted with dimethylsilylene bis indene dilithium salt to give dimethylsilylene bis (1-indenyl) zirconium (N-methylanilide) chloride.

IC ICM C07F017-00

CC 35-3 (Chemistry of Synthetic High Polymers)
 Section cross-reference(s): 29, 67

L105 ANSWER 6 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 6

ACCESSION NUMBER: 1999:431903 HCAPLUS

DOCUMENT NUMBER: 131:87713

TITLE: Preparation of ruthenium-phosphine-amine complexes and stereoselective hydrogenation of carbonyl compounds to optically active alcohols using the complexes

INVENTOR(S): Ikariya, Takao; Ikehira, Hideyuki;
 Murata, Kunihiro; Kiyofuji, Nobuo;
 Ooka, Koji; Hashiguchi, Shohei; Okuma, Takeshi; Noyori, Ryoji

PATENT ASSIGNEE(S): Foundation for Scientific Technology
 Promotion, Japan; Nippon Kokan Co., Ltd.;
 Sumitomo Chemical Co., Ltd.; Kanto
 Kagaku K. K.; Takasago Perfumery Co.,
 Ltd.; Nippon Soda Co., Ltd.; Takeda Chemical
 Industries, Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189600	A2	19990713	JP 1997-359654	1997 1226

PRIORITY APPLN. INFO.: JP 1997-359654
 1997

1226

OTHER SOURCE(S): CASREACT 131:87713; MARPAT 131:87713

ED Entered STN: 14 Jul 1999

AB Ruthenium-phosphine-amine complexes represented by formula
RuXY(PR1R2R3)n(NR6R7R8)m [I; X, Y = H, halo, CO2H, other anion; R1
- R3 = (un)substituted hydrocarbyl; or R1 and R2 are linked
together to form an (un)substituted carbocyclic ring; n = 0-4; R6
- R8 = H, (un)substituted hydrocarbyl; m = 0-4],
RuXY(PR1R2R3)n(R6R7N-Z-NR9R10)m [II; X, Y, R1 - R3, m = defined in
I; R6, R7, R9, R10 = H, (un)substituted hydrocarbyl; Z =
(un)substituted hydrocarbyl], RuXY(PR1R2-W-PR4R5)n(NR6R7R8)m [III;
X, Y, R6 - R8, n, m = defined in I; R1 - R5 = (un)substituted
hydrocarbyl or R1 and R2 or R4 and R5 are linked together to form
a (un)substituted carbocyclic ring; W = (un)substituted
hydrocarbyl], or RuXY(PR1R2-W-PR4R5)n(R6R7N-Z-NR9R10)m (X, Y, R1
- R5, n, m = defined in III; R6, R7, R9, R10 = defined in II) are
prepared. Optically active alcs., useful as intermediates for drugs,
agrochems., or many commonly used chems., are prepared in high
yields and high selectivity by reduction of carbonyl compds. with
hydrogen or hydrogen-donating compound in the presence of the above
ruthenium-phosphine-amine catalysts. Thus, 534 mg
[RuCl2(S)-BINAP](DMF)n, 1.117 mg (S,S)-1,2-diphenylethylenediamine
(DPEN), and 15 mL DMF were stirred at room temperature under Ar
overnight and cooled to -50°. The precipitated crystals were
recrystd. from toluene/hexane to give 361 mg [(S)-BINAP]RuCl2
(S,S)-DPEN (IV). IV (12.2 mg) and 11.5 mg KOCMe3 were dissolved
in 5 mL 2-propanol, placed in an autoclave under Ar, and stirred
for 30 min. Acetophenone (600 mg) was added and the resulting
mixture was pressurized by hydrogen to 3 atm and hydrogeanted under
stirring for 50 min to give ≥99% (R)-1-phenethyl alc. of
81.7% ee.

IC ICM C07F015-00

ICS B01J031-24; C07C029-145; C07C033-22; C07B061-00; C07M007-00

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)
Section cross-reference(s): 67, 78

L105 ANSWER 7 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 7

ACCESSION NUMBER: 1999:431891 HCAPLUS

DOCUMENT NUMBER: 131:87717

TITLE: Preparation of alcohols by catalytic
hydrogenation of carbonyl compounds

INVENTOR(S): Ikehira, Hideyuki; Murata, Kunihiko;
Ikariya, Takao; Okuma, Takeshi;
Noyori, Ryoji

PATENT ASSIGNEE(S): Foundation for Scientific Technology
Promotion, Japan; Sumitomo Chemical Co., Ltd.;
Kanto Kagaku K. K.; Nippon
Kokan Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189559	A2	19990713	JP 1997-359656	

1997
1226

PRIORITY APPLN. INFO.:

JP 1997-359656

1997
1226

OTHER SOURCE(S): CASREACT 131:87717; MARPAT 131:87717

ED Entered STN: 14 Jul 1999

AB Alcs. represented by formula $R_1CH(OH)R_2$ [$R_1, R_2 = H, \text{halo},$
(un)substituted hydrocarbyl or heterocyclyl, RO, RO_2C ; $R =$
(un)substituted hydrocarbyl or heterocyclyl; or R_1 and R_2 are
linked together to form a ring provided that R_1 and R_2 are not
halogen atoms] are prepared by hydrogenation of carbonyl compds.
represented by formula R_1COR_2 ($R_1, R_2 = \text{same as above}$) in the
presence of a homogeneous hydrogenation catalyst, N-containing organic
compound, and base in liquid reaction medium. The homogeneous
catalyst is a transition metal catalyst of group VIII metals in
particular rhodium, ruthenium, iridium, and platinum, whereas base
is an alkali or alkaline earth metal hydroxide or salt or a quaternary
ammonium salt. This process uses inexpensive and practical
ruthenium complexes of high activity and can rapidly hydrogenate
carbonyl compds. to alcs. in high yields which are intermediates
for drugs, agrochems., and many commonly used chems. Thus,
[$RuCl_2(cod)$]2 0.01, KOH 0.04, ethylenediamine 0.02, and
benzophenone 5.0 mmol were dissolved in 10 mL 2-propanol, 2 mL
PhMe, and 100 μ L DMF and hydrogenated in an 100 mL metal
autoclave at hydrogen pressure of 40 atm under stirring for 3 h to
give $\geq 99\%$ benzhydrol (Ph_2CHOH).

IC ICM C07C033-18

ICS B01J031-22; C07B041-02; C07C029-145; C07C031-125; C07C035-08;
C07B061-00CC 25-16 (Benzene, Its Derivatives, and Condensed Benzenoid
Compounds)

L105 ANSWER 8 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 8

ACCESSION NUMBER: 1999:439512 HCAPLUS

DOCUMENT NUMBER: 131:87714

TITLE: Preparation of optical active alcohols by
asymmetric hydrogenation of carbonyl compoundsINVENTOR(S): Ikehira, Hideyuki; Murata, Kunihiro;
Ikariya, Takao; Ohkuma, Takeshi;
Noyori, RyojiPATENT ASSIGNEE(S): Foundation for Scientific Technology
Promotion, Japan; Sumitomo Chemical Co., Ltd.;
Kanto Kagaku K. K.; Nippon
Kokan Co., Ltd.

SOURCE: Jpn. Kokai Tokkyo Koho, 8 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 11189558	A2	19990713	JP 1997-359655	

1997
1226

PRIORITY APPLN. INFO.:

JP 1997-359655

1997
1226

OTHER SOURCE(S): CASREACT 131:87714; MARPAT 131:87714

ED Entered STN: 19 Jul 1999

AB Optically active alcs. represented by formula R1CHR2OH [R1, R2 = H, halo, (un)substituted hydrocarbyl or heterocyclyl, RO, RO2C; wherein R = (un)substituted hydrocarbyl or heterocyclyl; or R1 and R2 are linked to each other to form a ring constituting an sym. compound] are prepared by stereoselective hydrogenation of carbonyl compds. represented by formula R1COR2 (R1, R2 = same as above) in the presence of a transition metal catalyst, an optically active N-containing compound (in particular optically active amine), and base. This process can also easily recover catalysts in an industrial scale and gives in high yields optically active alcs. of high purity which are useful as liquid crystals or intermediates for drugs. Thus, a 0.5 M KOH solution in 2-propanol (120 μ L), 8.5 mg (S,S)-diphenylethylenediamine, 502 mg 2,4'-dichlorobenzophenone, 15 mL 2-propanol, and 4 mL toluene were placed in a reaction tube under Ar, followed by adding 6.1 mg [RuCl2(p-cymene)]2 after degassing-purging with Ar. The resulting solution was repeatedly degassed and purged with Ar, transferred to a metal autoclave and pressurized with hydrogen to 40 atm and stirred at 28° for 4 h to give (+)-2,4'-dichlorobenzhydrol of 45% ee.

IC ICM C07C033-18
ICS B01J031-22; C07B041-02; C07B053-00; C07C029-145; C07C033-46; C07B061-00; C07M007-00

CC 25-7 (Benzene, Its Derivatives, and Condensed Benzenoid Compounds)

L105 ANSWER 9 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 9

ACCESSION NUMBER: 1998:115900 HCAPLUS

DOCUMENT NUMBER: 128:154227

TITLE: Preparation of metallocene compounds

INVENTOR(S): Tsutsumi, Kunihiro; Hori, Junichi; Yamazaki, Yasuhiro; Sugawara, Yasuaki; **Murata, Kunihiro**; Yoshida, Masahiro

PATENT ASSIGNEE(S): **Kanto Kagaku**, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 4 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10045786	A2	19980217	JP 1996-218089	1996 0801
PRIORITY APPLN. INFO.:				1996 0801

OTHER SOURCE(S): CASREACT 128:154227

ED Entered STN: 26 Feb 1998

AB Characterized is a process for preparation of the title compds. (I) by treatment of cyclopentadiene, indene, fluorene, or bridged compds. thereof with alkyl lithium and reacted with transition metal salts. I, useful as catalysts in the production of polyolefin, are

prepared in an industrial manner efficiently and economically. Thus, 1,1-cyclopentadienyl-(9-fluorenyl)diphenylmethane was treated with n-BuLi in a mixture of toluene and THF, and further reacted with zirconium chloride to give 81% diphenylmethylene (9-fluorenyl) (cyclopentadiene) zirconium chloride.

IC ICM C07F017-00
CC 29-10 (Organometallic and Organometalloidal Compounds)
Section cross-reference(s): 78

L105 ANSWER 10 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 10
ACCESSION NUMBER: 1998:68511 HCAPLUS
DOCUMENT NUMBER: 128:167201
TITLE: Preparation of alkylcyclopentadienes as precursors for hydrogenation and olefin polymerization catalysts
INVENTOR(S): Murata, Kunihiro; Tsutsumi, Kunihiro; Yamaguchi, Hiroyuki; Yoshida, Masahiro
PATENT ASSIGNEE(S): Kanto Kagaku, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 10025258	A2	19980127	JP 1996-200974	1996 0712
PRIORITY APPLN. INFO.:			JP 1996-200974	1996 0712

OTHER SOURCE(S): CASREACT 128:167201; MARPAT 128:167201
ED Entered STN: 05 Feb 1998
AB Alkylcyclopentadienes are prepared by reaction of cyclopentadienes with (slightly) ≤ 1 equivalent mol alkyl lithium and alkylation with RX (R = C1-15 hydrocarbon; X = tosyl, mesyl, halo) in dipolar aprotic solvents. Cyclopentadiene was condensed with BuLi in hexane-THF at room temperature for 3 h and alkylated with BuBr in 1,3-dimethyl-2-imidazolidinone at room temperature for overnight to give 81% n-butylcyclopentadiene (I). I was condensed with BuLi in hexane-toluene at room temperature for 3 h and reacted with ZrCl₄ under reflux for 3 h to give 71% dichlorobis(n-butylcyclopentadienyl)zirconium.
IC ICM C07C013-15
ICS C07C002-86; C07C013-465
CC 24-4 (Alicyclic Compounds)
Section cross-reference(s): 35

L105 ANSWER 11 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 11
ACCESSION NUMBER: 1998:228999 HCAPLUS
DOCUMENT NUMBER: 128:270734
TITLE: Transition-metal containing organic compounds and their use as catalysts for olefin polymerization
INVENTOR(S): Murata, Kunihiro; Hori, Junichi;

PATENT ASSIGNEE(S): Yoshida, Masahiro
SOURCE: Kanto Kagaku K. K., Japan
Eur. Pat. Appl., 12 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
-----	----	-----	-----	
EP 834515	A2	19980408	EP 1997-116930	1997 0930
EP 834515	A3	19991124		
EP 834515	B1	20040225		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
JP 10109995	A2	19980428	JP 1996-281643	1996 1004
JP 3566819	B2	20040915		
US 5859276	A	19990112	US 1997-935422	1997 0923
PRIORITY APPLN. INFO.:				1996 1004
				JP 1996-281643 A

OTHER SOURCE(S): MARPAT 128:270734

ED Entered STN: 23 Apr 1998

AB Metallocene dichlorides were prepared E.g., bis(N-methylanilido)zirconium dichloride-2THF, prepared in 79% yield from PhNHMe and ZrCl₄ in THF, was complexed with 1,2-di-3-indenylethane to give 98% ethylenedi-1-indenylzirconium bis(N-methylanilide), which was chlorinated with gaseous HCl in CH₂Cl₂ to give 62% ethylenedi-1-indenylzirconium dichloride. Similarly prepared was 51% ethylenedi-1-indenylhafnium dichloride.

IC ICM C07F017-00

ICS C08F010-00; C07F007-00

CC 29-10 (Organometallic and Organometalloidal Compounds)

L105 ANSWER 12 OF 18 HCAPLUS COPYRIGHT 2006 ACS on STN DUPLICATE 12

ACCESSION NUMBER: 1998:228998 HCAPLUS

DOCUMENT NUMBER: 128:270733

TITLE: Process for synthesizing metallocene compounds

INVENTOR(S): Murata, Kunihiko; Hori, Junichi;

Yoshida, Masahiro

PATENT ASSIGNEE(S): Kanto Kagaku K. K., Japan

SOURCE: Eur. Pat. Appl., 19 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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EP 834514 A2 19980408 EP 1997-116929 1997
0930

EP 834514 A3 19991124
EP 834514 B1 20031022
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE,
MC, PT, IE, FI

JP 10109996 A2 19980428 JP 1996-281644 1996
1004

JP 3694371 B2 20050914
US 5892075 A 19990406 US 1997-936169 1997
0923

PRIORITY APPLN. INFO.: JP 1996-281644 A 1996
1004

OTHER SOURCE(S): MARPAT 128:270733

ED Entered STN: 23 Apr 1998

AB The object of the invention resides in the development of an improved process for synthesizing metallocene compds. useful as olefin polymerization catalysts. E.g., bis(N-methylanilido)zirconium dichloride-2THF, prepared in 79% yield from PhNHMe and ZrCl₄ in THF, was complexed with 1,2-di-3-indenylethane to give 98% ethylenedi-1-indenylzirconium bis(N-methylanilide), which was chlorinated with gaseous HCl in CH₂Cl₂ to give 62% ethylenedi-1-indenylzirconium dichloride. Similarly prepared was 51% ethylenedi-1-indenylzirconium dichloride.

IC ICM C07F017-00

CC 29-10 (Organometallic and Organometalloidal Compounds)

=> d 1105 13-18 iall abeq tech abex

YOU HAVE REQUESTED DATA FROM FILE 'HCAPLUS, WPIX' - CONTINUE? (Y)/N:y

L105 ANSWER 13 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN

ACCESSION NUMBER: 2005-653595 [67] WPIX

DOC. NO. CPI: C2005-197673 [67]

TITLE: Manufacture of optically active alcohol containing nitrogen-containing heterocyclic ring, involves reacting specific asymmetric metal complex and hydrogen donor

DERWENT CLASS: B03; C02

INVENTOR: KATAYAMA T; MURATA K

PATENT ASSIGNEE: (KAKA-C) KANTO KAGAKU KK

COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2005263662	A	20050929	(200567)*	JA	53 [0]	C07D211-14

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
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JP 2005263662 A

JP 2004-76676 20040317

PRIORITY APPLN. INFO: JP 2004-76676 20040317

INT. PATENT CLASSIF.:

MAIN: C07D211-14

SECONDARY: C07D401-04

BASIC ABSTRACT:

JP 2005263662 A UPAB: 20051223

NOVELTY - An asymmetric metal complex obtained by reacting optically active nitrogen compound, 8th group metallic compound and ketone compound, with salt of nitrogen-containing heteroaromatic compound, is subjected to hydrogen donor reaction, to obtain optically active alcohol containing nitrogen-content heterocyclic ring.

DETAILED DESCRIPTION - An asymmetric metal complex obtained by reacting optically active nitrogen compound of formula (2), 8th group metallic compound and ketone compound, with salt of nitrogen-containing heteroaromatic compound of formula (1), is subjected to hydrogen donor reaction, to obtain optically active alcohol containing nitrogen-content heterocyclic ring of formula (3) and/or (4).

R1-R4=complex monocyclic ring or complex polycyclic groups having saturated or unsaturated optionally substituted aliphatic hydrocarbon, optionally substituted aromatic monocyclic ring or aromatic polynuclear hydrocarbon group or optionally substituted alicyclic hydrocarbon group;

R2=H, halogen, carboxyl group, amino group, amide, hydroxyl, alkoxy or allyloxy;

X=halogen anion, borate anion, phosphate anion, sulfonate anion or carboxylate anion;

m,n=0-5;

R5=H or optionally substituted alkyl group;and

R6=alkyl group, optionally substituted aromatic monocyclic ring or aromatic polynuclear hydrocarbon group, saturated or unsaturated hydrocarbon or alicyclic hydrocarbon.

USE - As synthetic intermediate, catalyst for asymmetric synthesis, bioactive substance, beta-adrenergic effect blocker, pharmaceutical and agrochemical intermediate.

ADVANTAGE - An optically active alcohol is manufactured by an efficient method.

MANUAL CODE: CPI: B07-D05; B14-J02D2; C07-D05; C14-J02D2;
N02-E01

TECH

INORGANIC CHEMISTRY - Preferred Compound: The metallic compound is ruthenium compound.

ORGANIC CHEMISTRY - Preferred Compound: The metallic compound is ruthenium compound.

ORGANIC CHEMISTRY - Preferred Compound: The hydrogen donor is formic acid, formate or alcohol compound. Preferred Method: A base selected from organic amine, alkali metal hydroxide or alkali metal alkoxide, is used as base during manufacture of optically active alcohol.

ABEX DEFINITIONS - Preferred Definitions: - m,n=1; - R1=optionally substituted phenyl preferably 4-cyano phenyl group; - R2=optionally substituted dihydropyridazyl group preferably 4-oxo dihydro pyridazyl group; - R3=group of formula (5); - R4=group of formula (6); - R6=group of formula (7); - R7-R9=H, 1-8C alkyl, halogen atom or 1-8C alkoxy;and - p,q,o=1-5. - R3 and R4 mutually bonds to form a group of formula (8).

SPECIFIC COMPOUNDS - About 300 metallic compounds are disclosed

such as chloro((S,S)-N-(p-toluene sulfonyl)-1,2-diphenyl ethylene diamine) (benzene) ruthenium.

EXAMPLE - 1-(4-cyano phenyl carbonyl methyl)-4-(4,5-dihydropyridazine-3 (2H)-one-6-yl) pyridinium bromide (in g) (3.50), triethyl amine (9.6 ml), formic acid (4.4 ml), asymmetric metal complex (chloro((S,S)-N-(p-toluene sulfonyl)-1,2-diphenyl ethylene diamine) (mesitylene) ruthenium (27.6 mg), were stirred at 40degreesC for 24 hours in a flask. Saturated sodium hydrogen carbonate aqueous solution was added to the reaction liquid. The precipitated powder was filter separated. (R)-6-(1-(2-(4-cyano phenyl)-2-hydroxyethyl)-1,2,5,6-tetrahydro pyrido-4-yl)-4,5-dihydropyridazine-3 (2H)-one of 94% yield and 91% optical purity, was obtained.

L105 ANSWER 14 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2004-272579 [26] WPIX
DOC. NO. CPI: C2004-105911 [26]
TITLE: Preparation of aryloxy metallocene compounds such as racemic-ethylene bis(indenyl)zirconium bisphenoxide, useful in polymerization catalyst, involves simple aroxylation reaction
DERWENT CLASS: A17; E11; E12
INVENTOR: HORI J; MURATA K
PATENT ASSIGNEE: (KAKA-C) KANTO KAGAKU KK
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2003231693	A	20030819	(200426)*	JA	19[0]	C07F017-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2003231693 A		JP 2002-26362	20020204

PRIORITY APPLN. INFO: JP 2002-26362 20020204

INT. PATENT CLASSIF.:

MAIN: C07F017-00

SECONDARY: C07F007-00; C07F007-28

BASIC ABSTRACT:

JP 2003231693 A UPAB: 20050528

NOVELTY - An aryloxy metallocene compound such as racemic-ethylene bis(indenyl)zirconium bisphenoxide, racemic-ethylene bis(indenyl)zirconium bis(p-methoxy phenoxide), racemic-ethylene bis(indenyl)zirconium bis(o-phenyl phenoxide) or racemic-ethylene bis(indenyl)zirconium bis(p-methyl phenoxide) is prepared by a simple aroxylation reaction.

DETAILED DESCRIPTION - Preparation of compounds of formula (I) involves reacting compounds of formula (II) and ((III).

L1 and L2 = 1-20C aliphatic hydrocarbon (which may also contain a halogen atom, an oxygen atom, a silicon atom or a germanium atom) or 6-14C aromatic hydrocarbon, cyclopentadienyl, indenyl, tetrahydro indenyl, benzo indenyl, dibenzo indenyl, naphth indenyl, fluorenyl or azulenyl radical optionally joined together through hydrocarbon group, silicon atom or germanium atom;

M = titanium, zirconium or hafnium atom;

X = an oxygen atom or a sulfur atom;

R3-R7 = 1-12C oxygenated organic radical, a hydrogen atom, 1-20C hydrocarbon group, 6-14C aromatic hydrocarbon radical or a halogen atom, or join together to form an aliphatic or aromatic ring.

R1 and R2 = 1-14C aliphatic hydrocarbon or aromatic hydrocarbon radical optionally containing silicon or germanium. R1 and R2 may form a ring containing one or more nitrogen atoms.

USE - The aryloxy metallocene compound is used in polymerization catalysts.

ADVANTAGE - The aryloxy metallocene compound is produced by a cost-effective and simple method. The method avoids use of harmful chemicals which affect environment.

MANUAL CODE: CPI: A02-A06E1; E05-E; E05-E01; E05-F02; E05-L01; E05-M; E05-N

L105 ANSWER 15 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2003-868757 [81] WPIX
DOC. NO. CPI: C2003-245785 [81]
TITLE: New optically active diphosphine compound used as catalyst ligand for asymmetric synthesis reactions
DERWENT CLASS: E11; E19; J04
INVENTOR: IKARIYA T; MURATA K; OTA T; TSUTSUMI K
PATENT ASSIGNEE: (KAKA-C) KANTO KAGAKU KK
COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 2003206295	A	20030722	(200381)*	JA	13 [0]	C07F009-50

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 2003206295	A	JP 2001-401157	20011228

PRIORITY APPLN. INFO: JP 2001-401157 20011228

INT. PATENT CLASSIF.:

MAIN: C07F009-50

BASIC ABSTRACT:

JP 2003206295 A UPAB: 20050531

NOVELTY - Optically active diphosphine compound (I) is new.

DETAILED DESCRIPTION - An optically active diphosphine compound of formula (I) is new.

R1, R2 = linear or cyclic 1-20C hydrocarbon optionally substituted, preferably methyl or phenyl;

R3, R4 = H or 1-3C hydrocarbon, preferably H; and

R5-R8 = 1-30C hydrocarbon, preferably phenyl, 4-tolyl or 3,5-xylyl.

At least one of R5-R8 is not phenyl.

An INDEPENDENT CLAIM is also included for manufacture of (I).

USE - Ligand for catalyst used in various asymmetric synthesis reactions.

ADVANTAGE - The optically active diphosphine compound

improves the activity of the catalyst. It is obtained efficiently and inexpensively. The manufacturing method has high conversion ratio and selectivity.

MANUAL CODE: CPI: E05-G02; E05-G03B; J04-E04; N05-E01; N06-E01
TECH

ORGANIC CHEMISTRY - Preparation (claimed): Preparation of the optically active diphosphine compound involves producing diaryl phosphine borane by reacting diaryl phosphite and dimethyl sulfide borane.

ABEX DEFINITIONS - Preferred Definitions: - R3 = H; and - R4 = H or methyl.

EXAMPLE - Magnesium (in g) (3.42) and a tetrahydrofuran solution of 5-bromo-m-xylene (25.47) are added to a flask substituted with argon gas. The mixture is stirred at 60 degrees C for 45 minutes. A tetrahydrofuran solution of diethyl phosphite (6 ml) is added in drops for 40 minutes at room temperature. The solution is then refluxed for 3 hours, and the reaction solvent is distilled. Ethyl acetate and hydrochloric acid (150 ml) are added to obtain a saturated salt solution. The salt solution is dried and purified to produce di-(3,5-xylyl) phosphite (A) (10.56). - (A) (2) is dissolved in diethyl ether (20 ml). Dimethyl sulfide borane (0.92) is added and stirred. The reaction solution is filtered, solvent is removed by distillation, and di-(3,5-xylyl) phosphine borane (B) (1.82) is formed. p-Tosyl chloride (3.55), pyridine (1.72 ml), methylene chloride (2 ml) and methylene chloride solution of (R,R)-3-methyl-2,4-pentanediol (5 ml) are reacted at room temperature. Ethyl acetate (60 ml) is added, and a saturated salt solution is obtained after washing. The obtained solution is dried and purified to obtain (S,S)-3-methyl-2,4-pentane di tosylate (C) (1.92). Product (B) (1.82), tetrahydrofuran (12 ml) and n-butyl lithium (4.55 ml) are stirred at room temperature. Subsequently, dimethylformamide solution of product (C) (1.08) and diethyl ether (60 ml) are added to reaction solution and stirred. The saturated salt solution obtained is dried and purified. (S,S)-3-methyl-2,4-bis(di-3,5-xylyl phosphino) pentane (638 mg) is obtained.

L105 ANSWER 16 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
ACCESSION NUMBER: 2003-543871 [52] WPIX
DOC. NO. CPI: C2003-147745 [52]
TITLE: New ruthenium complex, used as catalyst for preparing optically active alcohol compound
DERWENT CLASS: E19; J04
INVENTOR: IKARIYA T; KUNIHICO M; KUNIHICO T;
MURATA K; OTA T; TAKAO I; TAKESHI O;
TSUTSUMI K
PATENT ASSIGNEE: (KAKA-C) KANTO KAGAKU KK
COUNTRY COUNT: 33

PATENT INFORMATION:

PATENT NO	KIND DATE	WEEK	LA	PG	MAIN IPC
EP 1323724	A2 20030702	(200352)*	EN	28[0]	C07F015-00
CA 2414265	A1 20030628	(200353)	EN		C07F015-00
US 20030166978	A1 20030904	(200359)	EN		C07C029-14
JP 2003252884	A 20030910	(200361)	JA	21	C07F009-50
JP 3566955	B2 20040915	(200460)	JA	33	C07F009-50
US 6790973	B2 20040914	(200460)	EN		C07F015-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
EP 1323724	A2	EP 2002-28791	20021223
JP 2003252884	A	JP 2002-248058	20020828
JP 3566955	B2	JP 2002-248058	20020828
CA 2414265	A1	CA 2002-2414265	20021216
US 20030166978	A1	US 2002-330501	20021227
US 6790973	B2	US 2002-330501	20021227

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP 3566955	B2	JP 2003252884

Previous Publ

PRIORITY APPLN. INFO: JP 2002-248058 20020828
JP 2001-401170 20011228

INT. PATENT CLASSIF.:

MAIN: C07C029-14; C07F015-00; C07F009-50
SECONDARY: B01J023-46; B01J031-24; C07C213-00; C07C215-30;
C07C029-145; C07C031-125; C07C031-135;
C07C033-20; C07C033-22; C07C033-46; C07D213-30;
C07D307-12; C07D333-16
ADDITIONAL: C07B053-00; C07B061-00
INDEX: C07M007:00

BASIC ABSTRACT:

EP 1323724 A2 UPAB: 20050903
NOVELTY - A ruthenium complex (I) used as catalyst for preparing optically active alcohol compound is new.
DETAILED DESCRIPTION - A ruthenium complex of formula (I) is new:
R1, R2 = 1-20C substituted chain/cyclic hydrocarbon;
R3, R4 = H or 1-3C hydrocarbon;
R5-R8 = 1-30C substituted hydrocarbon; and
X, Y = H or anion.
When X and Y are bromine, R1 and R2 are methyl, and when R3 and R4 are hydrogen, 1 of R5-R8 is not phenyl.
INDEPENDENT CLAIMS are also included for:
(1) a ruthenium complex of formula RuXYAB (II); and
(2) a process for preparing an alcoholic compound comprising reducing a carbonyl compound with reaction of hydrogen or a compound donating hydrogen in presence of (I) or (II).
A = group of formula (III);
B = group of formula (IV);
R9-R16 = H or 1-30 substituted chain/cyclic hydrocarbon;
and
Z = 1-10C substituted/single bond chain/cyclic hydrocarbon.

USE - The invention is used as catalyst for preparing optically active alcohol compound (claimed). It is used as intermediate of pharmaceuticals, agricultural chemicals, or commodity chemicals.

ADVANTAGE - The invention has asymmetry on carbon and is easy to synthesize. It provides alcoholic compounds that are excellent in terms of reactivity and enantioselectivity in asymmetric hydrogenation of carbonyl compounds compared with conventional ruthenium complex catalyst.

MANUAL CODE: CPI: E05-G02; E05-G03B; E05-M; E10-E04F; E11-D; J04-E04; N05-B; N05-D; N05-E01; N07-B

TECH

ORGANIC CHEMISTRY - Preferred Compounds: A is TolsKEWPHOS:2,4-bis-(di-4-tolylphosphino)pentane; XylsKEWPHOS:2,4-bis-(di-3,5-xylylphosphino)pentane; 2,4-bis-(diphenylphosphino)-3-methylpentane; 2,4-bis-(di-4-tolylphosphino)-3-methylpentane; 2,4-bis-(di-3,5-xylylphosphino)-3-methylpentane; 1,3-bis-(diphenylphosphino)-1,3-diphenylpropane; 1,3-bis-(di-4-tolylphosphino)-1,3-diphenylpropane; 1,3-bis-(di-3,5-xylylphosphino)-1,3-diphenylpropane; 1,3-bis-(diphenylphosphino)-1,3-diphenyl-2-methylpropane; 1,3-bis-(di-4-tolylphosphino)-1,3-diphenyl-2-methylpropane; or 1,3-bis-(di-3,5-xylylphosphino)-1,3-diphenyl-2-methylpropane. B is diphenylethylenediamine or 1-isopropyl-2,2-di(p-methoxyphenyl)ethylenediamine.

Preferred Method: The complex is obtained by reacting RuXY (V) with compound (III).

ABEX DEFINITIONS - Preferred Definition: - R1, R2 = methyl; - R3, R4 = H; - R5-R8 = phenyl, 4-tolyl, or 3,5-xylyl, preferably phenyl; - R13, R15 = H; - R14, R16 = phenyl; - R13, R14 = isopropyl; - R15, R16 = 4-methoxyphenyl; - R9-R12 = H; and - Z = single bond.

EXAMPLE - (R)-DAIPEN of formula (a) (115 mg, 0.35 mmol) was added to RuBr2((S,S)-Tolskewphos) complex (316 mg, 0.35 mmol) and replaced with argon. Subsequently, the mixture was added with dimethylformamide (14 ml), degassed, and stirred at room temperature overnight. - After the reaction liquid was filtered through a glass filter packed with silica gel, the solvent was evaporated. - The residue was crystallized from methylene chloride/isopropyl ether to give RuBr2((S,S)-Tolskewphos)((R)-daipen) (246 mg, 66% yield). - The formed RuBr2((S,S)-Tolskewphos)((R)-daipen) (2.1 mg (0.002 mmol) was placed in a 100 ml autoclave, replaced with argon, and subsequently added with acetophenone (2.3 ml, 20 mmol), 0.01M KOC(CH₃)₃-2-propanol solution (8 ml, 0.08 mmol), degassed and replaced with argon. Hydrogen was introduced to a pressure of 9 atm and the reaction was started. - After the reaction mixture was stirred for 19 hours, the reaction pressure was returned to normal pressure, and the quantity and the optical purity of the produced phenylethyl alcohol was determined by gas chromatography on the reaction liquid. - All the reaction substrate was consumed and the yield of product was not less than 99%. Also, for the obtained phenylethyl alcohol, (R)-product was formed in a yield of 93.8%.

L105 ANSWER 17 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 2000-475385 [41] WPIX
 DOC. NO. CPI: C2000-142349 [41]
 TITLE: Preparation of alcohol under mild conditions e.g. by hydrogenating carbonyl compound in presence of bipyridyl derivative, transition metal complex and base
 DERWENT CLASS: B05; C03; E19
 INVENTOR: IKARIYA T; IKEHIRA H; KATAYAMA E; KOZAWA M; MURATA K; NOYORI R; OHKUMA T; OKUMA T; OZAWA M; YOKOZAWA T
 PATENT ASSIGNEE: (NISC-N) JAPAN SCI & TECHNOLOGY CORP; (KAGA-N) KAGAKU GIJUTSU SHINKO JIGYODAN; (KANT-N) KANTA CHEM CO INC; (KAKA-C) KANTO KAGAKU KK; (NIPS-C) NIPPON SODA CO; (NISC-C) NISSAN CHEM IND LTD; (SUMO-C) SUMITOMO CHEM CO LTD; (TAKS-C) TAKASAGO INT CORP; (TAKS-C) TAKASAGO PERFUMERY CO LTD

COUNTRY COUNT: 21

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
WO 2000035845	A1	20000622	(200041)*	JA	26[0]	C07C029-145
JP 2000178215	A	20000627	(200042)	JA	7	C07C029-145
EP 1142856	A1	20011010	(200167)	EN		C07C029-145
US 6476278	B1	20021105	(200276)	EN		C07C027-00

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
WO 2000035845	A1	WO 1999-JP7035	19991215
JP 2000178215	A	JP 1998-358034	19981216
EP 1142856	A1	EP 1999-959820	19991215
EP 1142856	A1	WO 1999-JP7035	19991215
US 6476278	B1	WO 1999-JP7035	19991215
US 6476278	B1	US 2001-868169	20011025

FILING DETAILS:

PATENT NO	KIND	PATENT NO
EP 1142856	A1	Based on WO 2000035845 A
US 6476278	B1	Based on WO 2000035845 A

PRIORITY APPLN. INFO: JP 1998-358034 19981216

INT. PATENT CLASSIF.:

MAIN: C07C027-00; C07C029-145
 SECONDARY: B01J031-22; C07C031-10; C07C033-20; C07C033-22;
 C07C033-30; C07C035-08
 ADDITIONAL: C07B061-00

BASIC ABSTRACT:

WO 2000035845 A1 UPAB: 20050411

NOVELTY - Preparation of an alcohol comprises:

(i) reacting a carbonyl compound with hydrogen in the presence of a bipyridyl derivative, Group VIII transition metal complex and base or

(ii) reducing a carbonyl compound in the presence of a bipyridyl derivative, Group VIII transition metal complex, base and alcoholic solvent.

USE - Used for preparing alcohols useful e.g. as intermediates for pharmaceuticals and pesticides.

ADVANTAGE - Process is simple and produces alcohols under mild conditions in high yields with little side product.

MANUAL CODE: CPI: B10-E04; C10-E04; E10-E04D; E10-E04E; E10-E04F

Member(0002)

ABEQ JP 2000178215 A UPAB 20050411

NOVELTY - Preparation of an alcohol comprises:

(i) reacting a carbonyl compound with hydrogen in the presence of a bipyridyl derivative, Group VIII transition metal complex and base or

(ii) reducing a carbonyl compound in the presence of a bipyridyl derivative, Group VIII transition metal complex, base and alcoholic solvent.

USE - Used for preparing alcohols useful e.g., as intermediates for pharmaceuticals and pesticides.
 ADVANTAGE - Process is simple and produces alcohols under mild conditions in high yields with little side product.

TECH

ORGANIC CHEMISTRY - Preferred process: Carbonyl compound of formula R_1COR_2 (I) is reacted in the presence of an alkali metal or alkaline earth metal hydroxide or a quaternary ammonium hydroxide, a metal complex of formula $M_1X_mL_n$ (II) and a bipyridyl compound of formula (III).
 $R_1, R_2 = H, \text{ halo, alkoxy, carbonyl or optionally substituted alkyl, aralkyl, aryl, alkenyl or alkoxy or}$
 $R_1 + R_2 = \text{cyclic group;}$
 $M_1 = \text{rhodium, ruthenium, iridium or platinum;}$
 $X = H, \text{ halo, carboxyl, alkoxy or OH;}$
 $L = \text{organic group;}$
 $m, n = 0-6 \text{ and}$
 $m + n = 6 \text{ or less;}$
 $R_3-R_9 = H, \text{ halo or optionally substituted alkyl, aralkyl, aryl or alkenyl.}$

ABEX EXAMPLE - Chloro(pentamethylcyclopentadiyl) (1,5-cyclooctanediene) ruthenium (3.8 mg), potassium hydroxide (3.1 mg), 2,2-bipyridyl (3.1 mg) and acetophenone (600.75 mg) in 2-propanol (10 ml) were heated in an autoclave under hydrogen at 28degreesC and 50 atmospheres pressure for 3 hours with stirring to give 1-phenolethanol in at least 99% yield. In a comparative example in the absence of bipyridyl, the yield was 97% with 3% impurities.

L105 ANSWER 18 OF 18 WPIX COPYRIGHT 2006 THE THOMSON CORP on STN
 ACCESSION NUMBER: 1991-278290 [38] WPIX
 DOC. NO. CPI: C1991-120791 [21]
 TITLE: Optically active fluoro-alcohol(s) - useful as intermediates for pharmaceuticals, agrochemicals or liquid crystals
 DERWENT CLASS: B05; C03; E16
 INVENTOR: FUJII T; FUKIAGE A; MURATA K; YOSHIDA M
 PATENT ASSIGNEE: (KAKA-C) KANTO KAGAKU KK
 COUNTRY COUNT: 1

PATENT INFORMATION:

PATENT NO	KIND	DATE	WEEK	LA	PG	MAIN IPC
JP 03184929	A	19910812	(199138)*	JA		
JP 2879456	B2	19990405	(199919)	JA	9	C07C031-38

APPLICATION DETAILS:

PATENT NO	KIND	APPLICATION	DATE
JP 03184929 A		JP 1989-323851	19891215
JP 2879456 B2		JP 1989-323851	19891215

FILING DETAILS:

PATENT NO	KIND	PATENT NO
JP.2879456 B2	Previous Publ	JP 03184929 A

PRIORITY APPLN. INFO: JP 1989-323851 19891215
INT. PATENT CLASSIF.:

MAIN: C07C031-38
SECONDARY: C07C029-40
ADDITIONAL: B01J031-02; C07B061-00

BASIC ABSTRACT:

JP 03184929 A UPAB: 20050502

Optically active fluoro-alcohols (I) are new. In (I), R1 = 1-18C alkyl; R2 = 1-18C alkyl; asterisk C = asymmetric carbon atom.

Production of (I) comprises reacting a fluoro-aldehyde R1-CHF-CH=O (II) with an organometallic reagent as an alkylating agent in the presence or absence of a catalyst. Examples of the organometallic reagents are alkyl magnesium, alkyl lithium, alkyl titanium, alkyl lead and alkyl zinc.

USE/ADVANTAGE - (I) is useful as an intermediate for pharmaceuticals, agrochemicals or functional materials (e.g. strong dielectric liquid crystals). @ (9pp Dwg.No.0/0)@

MANUAL CODE: CPI: B10-E04D; B11-B; C10-E04D; C11-B; E10-E04F; N06

Member(0002)

ABEQ JP 2879456 B2 UPAB 20050502

Optically active fluoro-alcohols (I) are new. In (I), R1 = 1-18C alkyl; R2 = 1-18C alkyl; asterisk C = asymmetric carbon atom.

Prodn. of (I) comprises reacting a fluoro-aldehyde R1-CHF-CH=O (II) with an organometallic reagent as an alkylating agent in the presence or absence of a catalyst. Examples of the organometallic reagents are alkyl magnesium, alkyl lithium, alkyl titanium, alkyl lead and alkyl zinc.

USE/ADVANTAGE - (I) is useful as an intermediate for pharmaceuticals, agrochemicals or functional materials (e.g. strong dielectric liquid crystals).

=> d his ful

(FILE 'HOME' ENTERED AT 09:16:37 ON 21 NOV 2006)

FILE 'HCAPLUS' ENTERED AT 09:17:08 ON 21 NOV 2006

E US20040176616/PN

L1 1 SEA ABB=ON PLU=ON US20040176616/PN
D ALL
SEL RN

FILE 'REGISTRY' ENTERED AT 09:19:43 ON 21 NOV 2006

L2 33 SEA ABB=ON PLU=ON (105-45-3/BI OR 105-53-3/BI OR
108-59-8/BI OR 1121-66-0/BI OR 126-39-6/BI OR 151600-50
-9/BI OR 154194-50-0/BI OR 160115-23-1/BI OR 164931-77-
5/BI OR 164931-78-6/BI OR 167316-27-0/BI OR 173837-41-7
/BI OR 188444-42-0/BI OR 193530-87-9/BI OR 194095-90-4/
BI OR 22748-16-9/BI OR 24347-58-8/BI OR 287493-81-6/BI
OR 287493-82-7/BI OR 568590-07-8/BI OR 569342-29-6/BI
OR 609-02-9/BI OR 67421-02-7/BI OR 724774-82-7/BI OR
724774-83-8/BI OR 724774-84-9/BI OR 725737-67-7/BI OR
725737-68-8/BI OR 725737-69-9/BI OR 725737-70-2/BI OR
725737-71-3/BI OR 930-30-3/BI OR 930-68-7/BI)
D SCAN

FILE 'STNGUIDE' ENTERED AT 09:20:12 ON 21 NOV 2006

FILE 'REGISTRY' ENTERED AT 09:45:35 ON 21 NOV 2006

L3 9 SEA ABB=ON PLU=ON L2 AND ?CYCLOPENT?/CNS
D SCAN
D 1-9 RN CN STR

L4 1 SEA ABB=ON PLU=ON 194095-90-4/RN
D SCAN
D CN
E "(+)-(R)-3-[BIS(METHOXYCARBONYL)METHYL]CYCLOPENTANONE
E "(+)-(R)-3-(BIS(METHOXYCARBONYL)METHYL)CYCLOPENTANONE
E "(+)-(R)-3-(BIS(ETHOXYCARBONYL)METHYL)CYCLOPENTANONE"
E "(+)-(R)-3-(BIS(METHOXYCARBONYL)METHYL)CYCLOPENTANONE

L5 1 SEA ABB=ON PLU=ON "(+)-(R)-3-(BIS(METHOXYCARBONYL)MET
HYL)CYCLOPENTANONE"/CN
D SCAN
E "PROPANEDIOIC ACID, [(1R)-3-OXOCYCLOPENTYL]-, DIETHYL
D SCAN L3
D SCAN L4

L6 2 SEA ABB=ON PLU=ON L3 AND ?DIETHYL?/CNS
D SCAN

L7 1 SEA ABB=ON PLU=ON 193530-87-9/RN
D SCAN
D CN
E HEXAMETHYLENE BENZENE/CN

FILE 'LREGISTRY' ENTERED AT 10:09:58 ON 21 NOV 2006

L8 STR

FILE 'REGISTRY' ENTERED AT 10:23:29 ON 21 NOV 2006

L9 28 SEA SSS SAM L8

FILE 'CASREACT' ENTERED AT 10:24:16 ON 21 NOV 2006

L10 STR L8
L11 5 SEA SSS SAM L10 (37 REACTIONS)
D SCAN

L12 FILE 'REGISTRY' ENTERED AT 10:35:31 ON 21 NOV 2006
6 SEA ABB=ON PLU=ON L2 AND 1/M
D SCAN

L13 FILE 'CASREACT' ENTERED AT 10:38:21 ON 21 NOV 2006
STR L10

L14 1 SEA SSS SAM L13 (14 REACTIONS)
D SCAN

L15 629 SEA SSS FUL L10 (2897 REACTIONS)
SAV L15 SHI806CASRCT/A

L16 266 SEA ABB=ON PLU=ON L15 AND L2
D SCAN L14
D QUE L14
D QUE STAT
D QUE STAT L14

L17 STR L13

L18 1 SEA SSS SAM L17 (14 REACTIONS)
D SCAN

L19 1 SEA SUB=L15 SSS SAM L17 (14 REACTIONS)
D SCAN

L20 7 SEA SUB=L15 SSS FUL L17 (31 REACTIONS)
D SCAN
D QUE STAT
SAV TEMP L20 SHI806CSRCTA/A

FILE 'ZCAPLUS' ENTERED AT 10:57:30 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 12:31:02 ON 21 NOV 2006
D SCAN L1

FILE 'ZCAPLUS' ENTERED AT 12:31:02 ON 21 NOV 2006
D QUE STAT L9

L21 FILE 'REGISTRY' ENTERED AT 12:40:02 ON 21 NOV 2006
SCR 1918 OR 2043 OR 1840 OR 1949 OR 2010

L22 30 SEA SSS SAM L8 NOT L21
D QUE STAT

L23 FILE 'LREGISTRY' ENTERED AT 12:42:18 ON 21 NOV 2006
STR L8

L24 FILE 'REGISTRY' ENTERED AT 12:43:54 ON 21 NOV 2006
19 SEA SSS SAM L23 NOT L21
D SCAN
D QUE

FILE 'LREGISTRY' ENTERED AT 12:46:30 ON 21 NOV 2006

FILE 'STNGUIDE' ENTERED AT 12:49:12 ON 21 NOV 2006
D QUE STAT
D COST

L25 FILE 'LREGISTRY' ENTERED AT 12:55:04 ON 21 NOV 2006
STR L23

L26 FILE 'REGISTRY' ENTERED AT 12:57:18 ON 21 NOV 2006
47 SEA SSS SAM L25 NOT L21
D QUE STAT

L27 12118 SEA SSS FUL L25 NOT L21

L28 15 SEA ABB=ON PLU=ON L2 AND L27
SAV TEMP L27 SHI806REG/A
D SAV

L29 18 SEA ABB=ON PLU=ON L2 NOT L28
D SCAN

FILE 'LREGISTRY' ENTERED AT 13:03:24 ON 21 NOV 2006

L30 STR L25

FILE 'REGISTRY' ENTERED AT 13:10:40 ON 21 NOV 2006

L31 50 SEA SUB=L27 SSS SAM L30

L32 2503 SEA SUB=L27 SSS FUL L30
SAV TEMP L27 SHI806REGA/A
D QUE STAT

L33 14 SEA ABB=ON PLU=ON L2 AND L32
D SCAN
D QUE STAT

FILE 'LREGISTRY' ENTERED AT 13:14:01 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 13:14:32 ON 21 NOV 2006
D SCAN L1

FILE 'LREGISTRY' ENTERED AT 13:14:32 ON 21 NOV 2006

L34 STR L30

FILE 'REGISTRY' ENTERED AT 13:17:50 ON 21 NOV 2006

L35 50 SEA SSS SAM L34

L36 50 SEA SSS SAM L34 NOT L21

FILE 'LREGISTRY' ENTERED AT 13:19:08 ON 21 NOV 2006

L37 STR

FILE 'REGISTRY' ENTERED AT 13:24:03 ON 21 NOV 2006

L38 SCR 1918 OR 2043 OR 1839 OR 1945 OR 2005

L39 50 SEA SSS SAM L37 NOT L38

L40 SCR 1918 OR 2043 OR 1839 OR 1944 OR 2005

L41 50 SEA SSS SAM L37 NOT L40

L42 6815 SEA SSS FUL L37 NOT L40
SAV TEMP L42 SHI806REGB/A

FILE 'HCAPLUS' ENTERED AT 13:30:04 ON 21 NOV 2006

FILE 'REGISTRY' ENTERED AT 13:30:23 ON 21 NOV 2006

L43 4 SEA ABB=ON PLU=ON L2 AND L42
D SCAN

FILE 'HCAPLUS' ENTERED AT 13:31:18 ON 21 NOV 2006

L44 52 SEA ABB=ON PLU=ON L28

L45 6470 SEA ABB=ON PLU=ON L43

L46 49 SEA ABB=ON PLU=ON L44 AND L45

L47 50 SEA ABB=ON PLU=ON L28/P

L48 4494 SEA ABB=ON PLU=ON L43/RACT

L49 47 SEA ABB=ON PLU=ON L48 AND L47

L50 1507 SEA ABB=ON PLU=ON L32/P

L51 31232 SEA ABB=ON PLU=ON L42/RACT

L52 266 SEA ABB=ON PLU=ON L50 AND L51
D SCAN L1
E ASYMMETRIC SYNTHESIS AND INDUCTION/CT
E E3+ALL

L53 E "ASYMMETRIC SYNTHESIS AND INDUCTION"+PFT,OLD,NT/CT
 QUE ABB=ON PLU=ON "ASYMMETRIC SYNTHESIS AND INDUCTION
 "+PFT,OLD,NT/CT
 E MICHAEL REACTION/CT
 E E3+ALL
 L54 QUE ABB=ON PLU=ON "MICHAEL REACTION"+PFT,OLD,NT/CT
 E MICHAEL REACTION CATALYSTS/CT
 E E3+ALL
 L55 QUE ABB=ON PLU=ON "MICHAEL REACTION CATALYSTS"+PFT,OL
 D,NT/CT
 L56 30 SEA ABB=ON PLU=ON L53 AND L52
 L57 21 SEA ABB=ON PLU=ON L56 AND (L54 OR L55)
 D SCAN
 L58 1 SEA ABB=ON PLU=ON L1 AND L57
 L59 5174 SEA ABB=ON PLU=ON L27/P
 L60 31232 SEA ABB=ON PLU=ON L42/RAC
 L61 1337 SEA ABB=ON PLU=ON L60 AND L53
 L62 176 SEA ABB=ON PLU=ON L61 AND (L54 OR L55)
 L63 92 SEA ABB=ON PLU=ON L62 AND L55

FILE 'REGISTRY' ENTERED AT 13:44:20 ON 21 NOV 2006

L64 744935 SEA ABB=ON PLU=ON ((FE OR CO OR NI OR RU OR RH OR PD
 OR OS OR IR OR PT) (L)N)/ELS
 L65 6 SEA ABB=ON PLU=ON L2 AND L64
 D SCAN
 L66 316118 SEA ABB=ON PLU=ON L64 AND 1-2/N
 L67 262888 SEA ABB=ON PLU=ON L66 AND 1/M
 L68 22790 SEA ABB=ON PLU=ON L67 AND 1/RU
 L69 80253 SEA ABB=ON PLU=ON L67 AND (1/OS OR 1/IR OR 1/PT OR
 1/PD)
 L70 159878 SEA ABB=ON PLU=ON L67 NOT (L68 OR L69)
 L71 76518 SEA ABB=ON PLU=ON L70 AND 1/FE
 SET DETAIL ON PERM
 L72 83360 SEA ABB=ON PLU=ON L67 NOT (L68 OR L69 OR L71)

FILE 'HCAPLUS' ENTERED AT 14:06:41 ON 21 NOV 2006

L73 QUE ABB=ON PLU=ON L68
 L74 QUE ABB=ON PLU=ON L69
 L75 QUE ABB=ON PLU=ON L71
 L76 QUE ABB=ON PLU=ON L72
 L77 QUE ABB=ON PLU=ON L73 OR L74 OR L75 OR L76
 L78 10 SEA ABB=ON PLU=ON L63 AND L77
 L79 1 SEA ABB=ON PLU=ON L1 AND L78
 D QUE
 L80 9613 SEA ABB=ON PLU=ON L27
 L81 50879 SEA ABB=ON PLU=ON L42
 D QUE
 L82 31 SEA ABB=ON PLU=ON L80 AND L81 AND L77
 D QUE
 L83 7 SEA ABB=ON PLU=ON L82 AND L53
 D QUE
 D QUE L32
 L84 1971 SEA ABB=ON PLU=ON L32
 L85 315 SEA ABB=ON PLU=ON L84 AND L42
 L86 14 SEA ABB=ON PLU=ON L85 AND L77

FILE 'STNGUIDE' ENTERED AT 14:21:41 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 14:21:47 ON 21 NOV 2006
 D SCAN

FILE 'STNGUIDE' ENTERED AT 14:22:02 ON 21 NOV 2006
D QUE STAT

FILE 'REGISTRY' ENTERED AT 14:25:13 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 14:25:15 ON 21 NOV 2006

L87 39 SEA ABB=ON PLU=ON L57 OR L78 OR L83 OR L86
L88 1 SEA ABB=ON PLU=ON L1 AND L87
D SCAN L87

FILE 'STNGUIDE' ENTERED AT 14:27:48 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 14:30:37 ON 21 NOV 2006

L89 62 SEA ABB=ON PLU=ON L87 OR L56 OR L82
L90 48 SEA ABB=ON PLU=ON L89 AND (L53 OR L54 OR L55)
L91 1 SEA ABB=ON PLU=ON L1 AND L90

FILE 'ZCAPLUS' ENTERED AT 14:32:11 ON 21 NOV 2006

L92 QUE ABB=ON PLU=ON PY<2005 OR PRY<2005 OR AY<2005 OR
MY<2005 OR REVIEW/DT

FILE 'HCAPLUS' ENTERED AT 14:39:30 ON 21 NOV 2006

L93 34 SEA ABB=ON PLU=ON L90 AND L92
D SCAN TI CC

FILE 'STNGUIDE' ENTERED AT 14:40:51 ON 21 NOV 2006

FILE 'HCAPLUS' ENTERED AT 14:41:26 ON 21 NOV 2006

D SCAN
L94 15 SEA ABB=ON PLU=ON L93 AND L53 AND L54 AND L55
L95 1 SEA ABB=ON PLU=ON L1 AND L94
D SCAN
D SCAN L94
L96 34 SEA ABB=ON PLU=ON L93 OR L94
L97 QUE ABB=ON PLU=ON (KANTO(W)KAGAKU?)/PA,CS,CO,SO
L98 QUE ABB=ON PLU=ON WATANABE M?/AU OR MURATA K?/AU OR
IKARIYA T?/AU
L99 12 SEA ABB=ON PLU=ON L97 AND L98
D SCAN
D SAV
SAV TEMP L96 SHI806HCP/A
SAV TEMP L99 SHI806HCPIN/A

FILE 'MEDLINE' ENTERED AT 14:56:18 ON 21 NOV 2006

L100 0 SEA ABB=ON PLU=ON L97 AND L98

FILE 'EMBASE' ENTERED AT 15:04:58 ON 21 NOV 2006

L101 0 SEA ABB=ON PLU=ON L97 AND L98

FILE 'BIOSIS' ENTERED AT 15:05:14 ON 21 NOV 2006

L102 0 SEA ABB=ON PLU=ON L97 AND L98

FILE 'WPIX, CONFSCI, PASCAL, TEMA, JICST-EPLUS, NTIS, JAPIO,
SCISEARCH' ENTERED AT 15:06:47 ON 21 NOV 2006

L103 18 SEA ABB=ON PLU=ON L97 AND L98
SET DETAIL ON PERM
L104 18 SEA ABB=ON PLU=ON L97 AND L98
D TRI 1-18

FILE 'HCAPLUS, WPIX' ENTERED AT 15:09:37 ON 21 NOV 2006
L105 18 DUP REM L99 L104 (12 DUPLICATES REMOVED)
ANSWERS '1-12' FROM FILE HCAPLUS
ANSWERS '13-18' FROM FILE WPIX

FILE 'HCAPLUS' ENTERED AT 15:10:33 ON 21 NOV 2006

FILE 'CAOLD' ENTERED AT 15:10:44 ON 21 NOV 2006
L106 816 SEA ABB=ON PLU=ON L27
L107 175 SEA ABB=ON PLU=ON L32
L108 1649 SEA ABB=ON PLU=ON L42
L109 21 SEA ABB=ON PLU=ON L106 AND L108
L110 6 SEA ABB=ON PLU=ON L108 AND L107
D SCAN L110
L111 21 SEA ABB=ON PLU=ON L109 OR L110
L112 120 SEA ABB=ON PLU=ON L68
L113 0 SEA ABB=ON PLU=ON L112 AND L111

FILE 'CASREACT' ENTERED AT 15:19:13 ON 21 NOV 2006
D QUE STAT L20
D QUE STAT L20
D QUE STAT L20
D L20 1-7 IALL HIT

FILE 'HCAPLUS' ENTERED AT 15:32:12 ON 21 NOV 2006
D QUE STAT L93
D L93 1-34 IBIB ABS ED HITSTR HITIND

FILE 'CAOLD' ENTERED AT 15:35:33 ON 21 NOV 2006
D QUE STAT L111
D QUE L111
D L111 1-21 IALL HITSTR HITIND
D QUE STAT L99
D QUE STAT L104
D QUE STAT L105

FILE 'HCAPLUS, WPIX' ENTERED AT 15:42:35 ON 21 NOV 2006
D L105 1-12 IBIB ED AB HITIND

FILE 'CAOLD' ENTERED AT 15:42:38 ON 21 NOV 2006

FILE 'HCAPLUS, WPIX' ENTERED AT 15:44:05 ON 21 NOV 2006
D L105 13-18 IALL ABEQ TECH ABEX

FILE 'CAOLD' ENTERED AT 15:44:10 ON 21 NOV 2006

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